Model for "D4h1"

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General Condition

- Basis type: `lgs`
- SAMB selection:
  - Type: `[Q, G]`
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: $[A_{1g}, A_{2g}, B_{1g}, B_{2g}, E_g, A_{1u}, A_{2u}, B_{1u}, B_{2u}, E_u]$
  - 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.: $[A_{1g}, A_{2g}, B_{1g}, B_{2g}, E_g, A_{1u}, A_{2u}, B_{1u}, B_{2u}, E_u]$
  - Spin (s): `[0, 1]`
- Site-cluster selection:
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: $[A_{1g}, A_{2g}, B_{1g}, B_{2g}, E_g, A_{1u}, A_{2u}, B_{1u}, B_{2u}, E_u]$
- Bond-cluster selection:
  - Type: `[Q, G, M, T]`
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: $[A_{1g}, A_{2g}, B_{1g}, B_{2g}, E_g, A_{1u}, A_{2u}, B_{1u}, B_{2u}, E_u]$
- Max. neighbor: `10`
- Search cell range: `(-2, 3), (-2, 3), (-2, 3)`
- Toroidal priority: `false`

Group and Unit Cell

- Group: SG No. 123 D_{4h}^1 $P4/mmm$ [tetragonal]
- Associated point group: PG No. 123 D_{4h} $4/mmm$ [tetragonal]
- Unit cell:
  $a =$ `1.00000`, $b =$ `1.00000`, $c =$ `1.50000`, $\alpha =$ `90.0`, $\beta =$ `90.0`, $\gamma =$ `90.0`
- Lattice vectors (conventional cell):
  $\boldsymbol{a}_1 =$ `[ 1.00000, 0.00000, 0.00000]`
  $\boldsymbol{a}_2 =$ `[ 0.00000, 1.00000, 0.00000]`
  $\boldsymbol{a}_3 =$ `[ 0.00000, 0.00000, 1.50000]`

Symmetry Operation

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	$\{1\|0\}$	2	$\{2_{001}\|0\}$	3	$\{4^{+}_{001}\|0\}$	4	$\{4^{-}_{001}\|0\}$	5	$\{2_{010}\|0\}$
6	$\{2_{100}\|0\}$	7	$\{2_{110}\|0\}$	8	$\{2_{1-10}\|0\}$	9	$\{-1\|0\}$	10	$\{m_{001}\|0\}$
11	$\{-4^{+}_{001}\|0\}$	12	$\{-4^{-}_{001}\|0\}$	13	$\{m_{010}\|0\}$	14	$\{m_{100}\|0\}$	15	$\{m_{110}\|0\}$
16	$\{m_{1-10}\|0\}$								

Harmonics

Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A_{1g})$	A_{1g}	0	Q, T	-	-	1
2	$\mathbb{Q}_2(A_{1g})$	A_{1g}	2	Q, T	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
3	$\mathbb{G}_0(A_{1u})$	A_{1u}	0	G, M	-	-	1
4	$\mathbb{G}_2(A_{1u})$	A_{1u}	2	G, M	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
5	$\mathbb{G}_4(A_{1u}, 1)$	A_{1u}	4	G, M	1	-	$\frac{\sqrt{21}\left(x^4-3x^2y^2-3x^2z^2+y^4-3y^2z^2+z^4\right)}{6}$
6	$\mathbb{G}_4(A_{1u}, 2)$	A_{1u}	4	G, M	2	-	$-\frac{\sqrt{15}\left(x^4-12x^2y^2+6x^2z^2+y^4+6y^2z^2-2z^4\right)}{12}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
7	$\mathbb{Q}_5(A_{1u})$	A_{1u}	5	Q, T	-	-	$\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$
8	$\mathbb{G}_1(A_{2g})$	A_{2g}	1	G, M	-	-	z
9	$\mathbb{G}_3(A_{2g})$	A_{2g}	3	G, M	-	-	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
10	$\mathbb{Q}_4(A_{2g})$	A_{2g}	4	Q, T	-	-	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
11	$\mathbb{Q}_1(A_{2u})$	A_{2u}	1	Q, T	-	-	z
12	$\mathbb{Q}_3(A_{2u})$	A_{2u}	3	Q, T	-	-	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
13	$\mathbb{G}_4(A_{2u})$	A_{2u}	4	G, M	-	-	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
14	$\mathbb{Q}_2(B_{1g})$	B_{1g}	2	Q, T	-	-	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
15	$\mathbb{G}_3(B_{1g})$	B_{1g}	3	G, M	-	-	$\sqrt{15}xyz$
16	$\mathbb{Q}_4(B_{1g})$	B_{1g}	4	Q, T	-	-	$\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$
17	$\mathbb{G}_2(B_{1u})$	B_{1u}	2	G, M	-	-	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
18	$\mathbb{Q}_3(B_{1u})$	B_{1u}	3	Q, T	-	-	$\sqrt{15}xyz$
19	$\mathbb{G}_4(B_{1u})$	B_{1u}	4	G, M	-	-	$\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$
20	$\mathbb{Q}_2(B_{2g})$	B_{2g}	2	Q, T	-	-	$\sqrt{3}xy$
21	$\mathbb{G}_3(B_{2g})$	B_{2g}	3	G, M	-	-	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
22	$\mathbb{G}_2(B_{2u})$	B_{2u}	2	G, M	-	-	$\sqrt{3}xy$
23	$\mathbb{Q}_3(B_{2u})$	B_{2u}	3	Q, T	-	-	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
24	$\mathbb{G}_4(B_{2u})$	B_{2u}	4	G, M	-	-	$-\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$
25	$\mathbb{G}_{1,1}(E_g)$	E_g	1	G, M	-	1	x
26	$\mathbb{G}_{1,2}(E_g)$					2	$-y$
27	$\mathbb{Q}_{2,1}(E_g)$	E_g	2	Q, T	-	1	$\sqrt{3}yz$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
28	$\mathbb{Q}_{2,2}(E_g)$					2	$\sqrt{3}xz$
29	$\mathbb{G}_{3,1}(E_g,1)$	E_g	3	G, M	1	1	$\frac{x(2x^2-3y^2-3z^2)}{2}$
30	$\mathbb{G}_{3,2}(E_g,1)$					2	$\frac{y(3x^2-2y^2+3z^2)}{2}$
31	$\mathbb{G}_{3,1}(E_g,2)$	E_g	3	G, M	2	1	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
32	$\mathbb{G}_{3,2}(E_g,2)$					2	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
33	$\mathbb{Q}_{4,1}(E_g,1)$	E_g	4	Q, T	1	1	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$
34	$\mathbb{Q}_{4,2}(E_g,1)$					2	$\frac{\sqrt{35}xz(x-z)(x+z)}{2}$
35	$\mathbb{Q}_{4,1}(E_g,2)$	E_g	4	Q, T	2	1	$\frac{\sqrt{5}yz(6x^2-y^2-z^2)}{2}$
36	$\mathbb{Q}_{4,2}(E_g,2)$					2	$-\frac{\sqrt{5}xz(x^2-6y^2+z^2)}{2}$
37	$\mathbb{Q}_{1,1}(E_u)$	E_u	1	Q, T	-	1	x
38	$\mathbb{Q}_{1,2}(E_u)$					2	y
39	$\mathbb{G}_{2,1}(E_u)$	E_u	2	G, M	-	1	$\sqrt{3}yz$
40	$\mathbb{G}_{2,2}(E_u)$					2	$-\sqrt{3}xz$
41	$\mathbb{Q}_{3,1}(E_u,1)$	E_u	3	Q, T	1	1	$\frac{x(2x^2-3y^2-3z^2)}{2}$
42	$\mathbb{Q}_{3,2}(E_u,1)$					2	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
43	$\mathbb{Q}_{3,1}(E_u,2)$	E_u	3	Q, T	2	1	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
44	$\mathbb{Q}_{3,2}(E_u,2)$					2	$\frac{\sqrt{15}y(x-z)(x+z)}{2}$
45	$\mathbb{G}_{4,1}(E_u,1)$	E_u	4	G, M	1	1	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$
46	$\mathbb{G}_{4,2}(E_u,1)$					2	$-\frac{\sqrt{35}xz(x-z)(x+z)}{2}$
47	$\mathbb{G}_{4,1}(E_u,2)$	E_u	4	G, M	2	1	$\frac{\sqrt{5}yz(6x^2-y^2-z^2)}{2}$
48	$\mathbb{G}_{4,2}(E_u,2)$					2	$\frac{\sqrt{5}xz(x^2-6y^2+z^2)}{2}$

Basis in full matrix

Table 3: dimension = 8

	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)
	0	$\lvert s, \uparrow\rangle$ @A(1)	1	$\lvert s, \downarrow\rangle$ @A(1)	2	$\lvert p_x, \uparrow\rangle$ @A(1)	3	$\lvert p_x, \downarrow\rangle$ @A(1)	4	$\lvert p_y, \uparrow\rangle$ @A(1)
	5	$\lvert p_y, \downarrow\rangle$ @A(1)	6	$\lvert p_z, \uparrow\rangle$ @A(1)	7	$\lvert p_z, \downarrow\rangle$ @A(1)				

Table 4: Atomic basis (orbital part only)

orbital	definition
$\lvert s\rangle$	1
$\lvert p_x\rangle$	x
$\lvert p_y\rangle$	y
$\lvert p_z\rangle$	z

SAMB

604 (all 604) SAMBs

- 'A' site-cluster : `A`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: `1a`

$\boxed{\text{z1}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$

- 'A' site-cluster : `A`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
  * wyckoff: `1a`

$\boxed{\text{z269}}$ $\mathbb{G}_2^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z270}}$ $\mathbb{G}_0^{(1,1;c)}(A_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z318}}$ $\mathbb{Q}_1^{(c)}(A_{2u}) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z319}}$ $\mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z359}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z403}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z443}}$ $\mathbb{Q}_{1,1}^{(c)}(E_u) = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$

$\boxed{\text{z444}}$ $\mathbb{Q}_{1,2}^{(c)}(E_u) = \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$

$\boxed{\text{z445}}$ $\mathbb{Q}_{1,1}^{(1,0;c)}(E_u) = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$

$\boxed{\text{z446}}$ $\mathbb{Q}_{1,2}^{(1,0;c)}(E_u) = \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$

$\boxed{\text{z447}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = \dfrac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$

$\boxed{\text{z448}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$

- 'A' site-cluster : `A`
  * bra: $\langle p_x, \uparrow|$, $\langle p_x, \downarrow|$, $\langle p_y, \uparrow|$, $\langle p_y, \downarrow|$, $\langle p_z, \uparrow|$, $\langle p_z, \downarrow|$
  * ket: $|p_x, \uparrow\rangle$, $|p_x, \downarrow\rangle$, $|p_y, \uparrow\rangle$, $|p_y, \downarrow\rangle$, $|p_z, \uparrow\rangle$, $|p_z, \downarrow\rangle$
  * wyckoff: `1a`

$\boxed{\text{z2}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z3}}$ $\mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z4}}$ $\mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z5}}$ $\mathbb{Q}_0^{(1,1;c)}(A_{1g}) = \mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z49}}$ $\mathbb{G}_1^{(1,0;c)}(A_{2g}) = \mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z77}}$ $\mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z78}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z114}}$ $\mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z115}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z147}}$ $\mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$

$\boxed{\text{z148}}$ $\mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$

$\boxed{\text{z149}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$

$\boxed{\text{z150}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$

$\boxed{\text{z151}}$ $\mathbb{G}_{1,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$

$\boxed{\text{z152}}$ $\mathbb{G}_{1,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$

- 'A'-'A' bond-cluster : `A;A_001_1`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: `2b@2f`

$\boxed{\text{z6}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z79}}$ $\mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z271}}$ $\mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z320}}$ $\mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z360}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z404}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z449}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z450}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

- 'A'-'A' bond-cluster : `A;A_001_1`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
  * wyckoff: `2b@2f`

$\boxed{\text{z7}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z8}}$ $\mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z9}}$ $\mathbb{Q}_0^{(1,0;c)}(A_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z50}}$ $\mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z51}}$ $\mathbb{G}_2^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z52}}$ $\mathbb{G}_0^{(1,1;c)}(A_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z80}}$ $\mathbb{G}_1^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z81}}$ $\mathbb{G}_1^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z82}}$ $\mathbb{G}_1^{(1,0;c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z116}}$ $\mathbb{Q}_1^{(c)}(A_{2u}) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z117}}$ $\mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = -\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z118}}$ $\mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z153}}$ $\mathbb{Q}_2^{(c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z154}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z155}}$ $\mathbb{Q}_2^{(1,0;c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z156}}$ $\mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z157}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z158}}$ $\mathbb{G}_2^{(1,1;c)}(B_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z159}}$ $\mathbb{Q}_2^{(c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z160}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z161}}$ $\mathbb{Q}_2^{(1,0;c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z162}}$ $\mathbb{Q}_3^{(c)}(B_{2u}) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z163}}$ $\mathbb{Q}_3^{(1,0;c)}(B_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z164}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z272}}$ $\mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_1^{(a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z273}}$ $\mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_1^{(a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z274}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$

$\boxed{\text{z321}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = -\frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$

$\boxed{\text{z322}}$ $\mathbb{Q}_{2,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z323}}$ $\mathbb{Q}_{2,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z361}}$ $\mathbb{G}_{1,1}^{(1,-1;c)}(E_g) = -\frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$

$\boxed{\text{z362}}$ $\mathbb{G}_{1,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$

$\boxed{\text{z363}}$ $$\mathbb{G}_{3,1}^{(1,-1;c)}(E_g,1) = \frac{\mathbb{M}_{2}^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\mathbb{M}_{2}^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z405}}$ $$\mathbb{G}_{3,2}^{(1,-1;c)}(E_g,1) = \frac{\mathbb{M}_{2}^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\mathbb{M}_{2}^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$\boxed{\text{z406}}$ $$\mathbb{G}_{1,1}^{(1,1;c)}(E_g) = \frac{\sqrt{2}\mathbb{M}_{0}^{(1,1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$\boxed{\text{z407}}$ $$\mathbb{G}_{1,2}^{(1,1;c)}(E_g) = -\frac{\sqrt{2}\mathbb{M}_{0}^{(1,1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z451}}$ $$\mathbb{Q}_{1,1}^{(c)}(E_u,a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z452}}$ $$\mathbb{Q}_{1,2}^{(c)}(E_u,a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z453}}$ $$\mathbb{Q}_{1,1}^{(c)}(E_u,b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}$$

$\boxed{\text{z454}}$ $$\mathbb{Q}_{1,2}^{(c)}(E_u,b) = -\frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}$$

$\boxed{\text{z455}}$ $$\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}$$

$\boxed{\text{z456}}$ $$\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}$$

$\boxed{\text{z457}}$ $$\mathbb{Q}_{1,1}^{(1,0;c)}(E_u,a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z458}}$ $$\mathbb{Q}_{1,2}^{(1,0;c)}(E_u,a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z459}}$ $$\mathbb{Q}_{1,1}^{(1,0;c)}(E_u,b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}$$

$\boxed{\text{z460}}$ $$\mathbb{Q}_{1,2}^{(1,0;c)}(E_u,b) = -\frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}$$

$\boxed{\text{z461}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z462}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

- 'A'-'A' bond-cluster : `A;A_001_1`
  - bra: $\langle p_x, \uparrow|$, $\langle p_x, \downarrow|$, $\langle p_y, \uparrow|$, $\langle p_y, \downarrow|$, $\langle p_z, \uparrow|$, $\langle p_z, \downarrow|$
  - ket: $|p_x, \uparrow\rangle$, $|p_x, \downarrow\rangle$, $|p_y, \uparrow\rangle$, $|p_y, \downarrow\rangle$, $|p_z, \uparrow\rangle$, $|p_z, \downarrow\rangle$
  - wyckoff: `2b@2f`

$\boxed{\text{z10}}$ $\mathbb{Q}_0^{(c)}(A_{1g}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z11}}$ $\mathbb{Q}_0^{(c)}(A_{1g}, b) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z12}}$ $\mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z13}}$ $\mathbb{Q}_0^{(1,-1;c)}(A_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z14}}$ $\mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z15}}$ $\mathbb{Q}_0^{(1,1;c)}(A_{1g}) = \mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z53}}$ $\mathbb{G}_0^{(c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z54}}$ $\mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z55}}$ $\mathbb{G}_2^{(1,-1;c)}(A_{1u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$

$\boxed{\text{z83}}$ $\mathbb{G}_4^{(1,-1;c)}(A_{1u}, 1) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$

$\boxed{\text{z84}}$ $\mathbb{G}_2^{(1,0;c)}(A_{1u}) = -\frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z85}}$ $\mathbb{G}_0^{(1,1;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$$\boxed{\text{z86}}\quad \mathbb{Q}_4^{(c)}(A_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z87}}\quad \mathbb{Q}_4^{(1,-1;c)}(A_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z88}}\quad \mathbb{G}_1^{(1,0;c)}(A_{2g}) = \mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z119}}\quad \mathbb{Q}_1^{(c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z120}}\quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z121}}\quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z165}}\quad \mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z166}}\quad \mathbb{Q}_1^{(1,1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z167}}\quad \mathbb{G}_4^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z168}}\quad \mathbb{Q}_2^{(c)}(B_{1g},a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z169}}\quad \mathbb{Q}_2^{(c)}(B_{1g},b) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z170}}\quad \mathbb{Q}_2^{(c)}(B_{1g},c) = -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z171}}\quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g},a) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z172}}\quad \mathbb{Q}_2^{(1,-1;c)}(B_{1g},b) = -\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z173}}\quad \mathbb{Q}_2^{(1,1;c)}(B_{1g}) = \mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z174}}\quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z175}}$ $\mathbb{Q}_3^{(1,0;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z176}}$ $\mathbb{G}_2^{(c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z275}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z276}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u}, b) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z277}}$ $\mathbb{G}_2^{(1,1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z278}}$ $\mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z279}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z280}}$ $\mathbb{Q}_2^{(1,0;c)}(B_{2g}) = \mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z324}}$ $\mathbb{Q}_3^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{30}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{30}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$

$\boxed{\text{z325}}$ $\mathbb{Q}_3^{(1,0;c)}(B_{2u}) = -\frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z326}}$ $\mathbb{G}_2^{(c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z327}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{2u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z328}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{2u}, b) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{30}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{30}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$

$\boxed{\text{z329}}$ $\mathbb{G}_2^{(1,1;c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z364}}$ $\mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z365}}$ $\mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z366}}$ $\mathbb{Q}_{2,1}^{(c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$

$\boxed{\text{z367}}$ $\mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$

$\boxed{\text{z368}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z369}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z408}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$

$\boxed{\text{z409}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$

$\boxed{\text{z410}}$ $\mathbb{Q}_{2,1}^{(1,0;c)}(E_g) = -\frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$

$\boxed{\text{z411}}$ $\mathbb{Q}_{2,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$

$\boxed{\text{z412}}$ $\mathbb{G}_{1,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z413}}$ $\mathbb{G}_{1,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z463}}$ $\mathbb{Q}_{1,1}^{(c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z464}}$ $\mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z465}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z466}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z467}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,1) = \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$

$\boxed{\text{z468}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,1) = -\frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$

$\boxed{\text{z469}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,2) = \frac{\sqrt{165}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{44} + \frac{2\sqrt{11}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{11} + \frac{3\sqrt{11}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{44}$

$\boxed{\text{z470}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,2) = -\frac{\sqrt{165}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{44} - \frac{2\sqrt{11}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{11} + \frac{3\sqrt{11}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{44}$

$\boxed{\text{z471}}$ $\mathbb{Q}_{1,1}^{(1,0;c)}(E_u) = -\frac{\sqrt{14}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{14}$

$\boxed{\text{z472}}$ $\mathbb{Q}_{1,2}^{(1,0;c)}(E_u) = -\frac{\sqrt{14}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{14}$

$\boxed{\text{z473}}$ $\mathbb{Q}_{3,1}^{(1,0;c)}(E_u,1) = -\frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{28} + \frac{3\sqrt{14}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{28} - \frac{\sqrt{14}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{7}$

$\boxed{\text{z474}}$ $\mathbb{Q}_{3,2}^{(1,0;c)}(E_u,1) = -\frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{28} - \frac{3\sqrt{14}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{28} - \frac{\sqrt{14}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{7}$

$\boxed{\text{z475}}$ $\mathbb{Q}_{3,1}^{(1,0;c)}(E_u,2) = -\frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$

$\boxed{\text{z476}}$ $\mathbb{Q}_{3,2}^{(1,0;c)}(E_u,2) = -\frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$

$\boxed{\text{z477}}$ $\mathbb{Q}_{1,1}^{(1,1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z478}}$ $\mathbb{Q}_{1,2}^{(1,1;c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z479}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{110}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{22} + \frac{\sqrt{66}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{22} - \frac{\sqrt{66}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{22}$

$\boxed{\text{z480}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{110}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{22} - \frac{\sqrt{66}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{22} - \frac{\sqrt{66}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{22}$

- 'A'-'A' bond-cluster : `A;A_002_1`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: `2c@1c`

$\boxed{\text{z16}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z122}}$ $\mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z281}}$ $\mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z330}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z370}}$ $\mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$

$\boxed{\text{z414}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z481}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z482}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

- 'A'-'A' bond-cluster : `A;A_002_1`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
  * wyckoff: `2c@1c`

$\boxed{\text{z17}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z18}}$ $$\mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z19}}$ $$\mathbb{Q}_0^{(1,0;c)}(A_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z56}}$ $$\mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{2g})$$

$\boxed{\text{z57}}$ $$\mathbb{G}_2^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$\boxed{\text{z58}}$ $$\mathbb{G}_0^{(1,1;c)}(A_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$\boxed{\text{z89}}$ $$\mathbb{G}_1^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$\boxed{\text{z90}}$ $$\mathbb{G}_1^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$\boxed{\text{z91}}$ $$\mathbb{G}_1^{(1,0;c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$\boxed{\text{z123}}$ $$\mathbb{Q}_1^{(c)}(A_{2u}) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$\boxed{\text{z124}}$ $$\mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{2g})$$

$\boxed{\text{z125}}$ $$\mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$\boxed{\text{z177}}$ $$\mathbb{Q}_2^{(c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z178}}$ $$\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z179}}$ $$\mathbb{Q}_2^{(1,0;c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z180}}$ $$\mathbb{Q}_3^{(c)}(B_{1u}) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{2g})$$

$\boxed{\text{z181}}$ $$\mathbb{Q}_3^{(1,0;c)}(B_{1u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{2g})$$

$\boxed{\text{z182}}$ $\mathbb{G}_{2}^{(1,-1;c)}(B_{1u}) = \mathbb{G}_{2}^{(1,-1;a)}(B_{1u})\mathbb{Q}_{0}^{(b)}(A_{1g})$

$\boxed{\text{z183}}$ $\mathbb{Q}_{2}^{(c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_{u})\mathbb{T}_{1,2}^{(b)}(E_{u})}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_{u})\mathbb{T}_{1,1}^{(b)}(E_{u})}{2}$

$\boxed{\text{z184}}$ $\mathbb{Q}_{2}^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_{u})\mathbb{T}_{1,2}^{(b)}(E_{u})}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_{u})\mathbb{T}_{1,1}^{(b)}(E_{u})}{2}$

$\boxed{\text{z185}}$ $\mathbb{Q}_{2}^{(1,0;c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_{u})\mathbb{T}_{1,2}^{(b)}(E_{u})}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_{u})\mathbb{T}_{1,1}^{(b)}(E_{u})}{2}$

$\boxed{\text{z186}}$ $\mathbb{Q}_{3}^{(1,-1;c)}(B_{2u}) = -\mathbb{G}_{2}^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2}^{(b)}(B_{2g})$

$\boxed{\text{z187}}$ $\mathbb{G}_{2}^{(1,-1;c)}(B_{2u}) = \mathbb{G}_{2}^{(1,-1;a)}(B_{2u})\mathbb{Q}_{0}^{(b)}(A_{1g})$

$\boxed{\text{z188}}$ $\mathbb{G}_{2}^{(1,1;c)}(B_{2u}) = \mathbb{G}_{0}^{(1,1;a)}(A_{1u})\mathbb{Q}_{2}^{(b)}(B_{2g})$

$\boxed{\text{z282}}$ $\mathbb{Q}_{2,1}^{(c)}(E_{g}) = \frac{\sqrt{2}\mathbb{T}_{1}^{(a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_{u})}{2}$

$\boxed{\text{z283}}$ $\mathbb{Q}_{2,2}^{(c)}(E_{g}) = \frac{\sqrt{2}\mathbb{T}_{1}^{(a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_{u})}{2}$

$\boxed{\text{z284}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E_{g}) = \frac{\sqrt{30}\mathbb{M}_{2}^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_{u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2}^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_{u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2}^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_{u})}{10}$

$\boxed{\text{z331}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E_{g}) = -\frac{\sqrt{30}\mathbb{M}_{2}^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_{u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2}^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_{u})}{10} - \frac{\sqrt{10}\mathbb{M}_{2}^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_{u})}{10}$

$\boxed{\text{z332}}$ $\mathbb{Q}_{2,1}^{(1,0;c)}(E_{g}) = \frac{\sqrt{2}\mathbb{T}_{1}^{(1,0;a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_{u})}{2}$

$\boxed{\text{z333}}$ $\mathbb{Q}_{2,2}^{(1,0;c)}(E_{g}) = \frac{\sqrt{2}\mathbb{T}_{1}^{(1,0;a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_{u})}{2}$

$\boxed{\text{z371}}$ $\mathbb{G}_{1,1}^{(1,-1;c)}(E_{g}) = -\frac{\sqrt{5}\mathbb{M}_{2}^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_{u})}{5} + \frac{\sqrt{15}\mathbb{M}_{2}^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_{u})}{10} + \frac{\sqrt{15}\mathbb{M}_{2}^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_{u})}{10}$

$\boxed{\text{z372}}$ $\mathbb{G}_{1,2}^{(1,-1;c)}(E_{g}) = \frac{\sqrt{5}\mathbb{M}_{2}^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_{u})}{5} + \frac{\sqrt{15}\mathbb{M}_{2}^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_{u})}{10} - \frac{\sqrt{15}\mathbb{M}_{2}^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_{u})}{10}$

$$\boxed{\text{z373}} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(E_g, 1) = \frac{\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z415}} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(E_g, 1) = \frac{\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z416}} \quad \mathbb{G}_{1,1}^{(1,1;c)}(E_g) = \frac{\sqrt{2}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z417}} \quad \mathbb{G}_{1,2}^{(1,1;c)}(E_g) = -\frac{\sqrt{2}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z483}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z484}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z485}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, b) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z486}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z487}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z488}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z489}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z490}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z491}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u, b) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z492}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$$

$\boxed{\text{z493}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z494}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

- 'A'-'A' bond-cluster : `A;A_002_1`
  - * bra: $\langle p_x,\uparrow|$, $\langle p_x,\downarrow|$, $\langle p_y,\uparrow|$, $\langle p_y,\downarrow|$, $\langle p_z,\uparrow|$, $\langle p_z,\downarrow|$
  - * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
  - * wyckoff: `2c@1c`

$\boxed{\text{z20}}$ $\mathbb{Q}_0^{(c)}(A_{1g},a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z21}}$ $\mathbb{Q}_0^{(c)}(A_{1g},b) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{2g})$

$\boxed{\text{z22}}$ $\mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z23}}$ $\mathbb{Q}_0^{(1,-1;c)}(A_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{2g})$

$\boxed{\text{z24}}$ $\mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z25}}$ $\mathbb{Q}_0^{(1,1;c)}(A_{1g}) = \mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z59}}$ $\mathbb{G}_0^{(c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z60}}$ $\mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z61}}$ $\mathbb{G}_2^{(1,-1;c)}(A_{1u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$

$\boxed{\text{z92}}$ $\mathbb{G}_4^{(1,-1;c)}(A_{1u},1) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$

$\boxed{\text{z93}}$ $\mathbb{G}_2^{(1,0;c)}(A_{1u}) = -\frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z94}}$ $\mathbb{G}_0^{(1,1;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z126}}$ $\mathbb{Q}_4^{(c)}(A_{2g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$

$\boxed{\text{z127}}$ $\mathbb{Q}_4^{(1,-1;c)}(A_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$

$\boxed{\text{z128}}$ $\mathbb{G}_1^{(1,0;c)}(A_{2g}) = \mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z129}}$ $\mathbb{Q}_1^{(c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z130}}$ $\mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z131}}$ $\mathbb{Q}_3^{(1,-1;c)}(A_{2u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$

$\boxed{\text{z189}}$ $\mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z190}}$ $\mathbb{Q}_1^{(1,1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z191}}$ $\mathbb{G}_4^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$

$\boxed{\text{z192}}$ $\mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z193}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z194}}$ $\mathbb{Q}_2^{(1,0;c)}(B_{1g}) = -\mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_2^{(b)}(B_{2g})$

$\boxed{\text{z195}}$ $\mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z196}}$ $\mathbb{Q}_3^{(1,0;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z197}}$ $\mathbb{G}_2^{(c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z198}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u},a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z199}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u},b) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z200}}$ $\mathbb{G}_2^{(1,1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z285}}$ $\mathbb{Q}_2^{(c)}(B_{2g},a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$

$\boxed{\text{z286}}$ $\mathbb{Q}_2^{(c)}(B_{2g},b) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z287}}$ $\mathbb{Q}_2^{(c)}(B_{2g},c) = -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$

$\boxed{\text{z288}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{2g},a) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z289}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{2g},b) = -\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$

$\boxed{\text{z290}}$ $\mathbb{Q}_2^{(1,1;c)}(B_{2g}) = \mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$

$\boxed{\text{z334}}$ $\mathbb{Q}_3^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{30}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{30}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$

$\boxed{\text{z335}}$ $\mathbb{Q}_3^{(1,0;c)}(B_{2u}) = -\frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z336}}$ $\mathbb{G}_2^{(c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z337}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{2u},a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z338}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{2u},b) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{30}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{30}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$

$\boxed{\text{z339}}$ $\mathbb{G}_2^{(1,1;c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z374}}$ $\mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z375}}$ $\mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z376}}$ $\mathbb{Q}_{2,1}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{2g})}{2}$

$\boxed{\text{z377}}$ $\mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{2g})}{2}$

$\boxed{\text{z378}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z379}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z418}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{2g})}{2}$

$\boxed{\text{z419}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{2g})}{2}$

$\boxed{\text{z420}}$ $\mathbb{Q}_{2,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{2g})}{2}$

$\boxed{\text{z421}}$ $\mathbb{Q}_{2,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{2g})}{2}$

$\boxed{\text{z422}}$ $\mathbb{G}_{1,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z423}}$ $\mathbb{G}_{1,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z495}}$ $\mathbb{Q}_{1,1}^{(c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1}^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z496}}$ $\mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_{1}^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z497}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z498}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z499}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,1) = \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$

$\boxed{\text{z500}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,1) = -\frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$

$\boxed{\text{z501}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,2) = \frac{\sqrt{165}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{44} + \frac{2\sqrt{11}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{11} + \frac{3\sqrt{11}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{44}$

$\boxed{\text{z502}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,2) = -\frac{\sqrt{165}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{44} - \frac{2\sqrt{11}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{11} + \frac{3\sqrt{11}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{44}$

$\boxed{\text{z503}}$ $\mathbb{Q}_{1,1}^{(1,0;c)}(E_u) = -\frac{\sqrt{14}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{14}$

$\boxed{\text{z504}}$ $\mathbb{Q}_{1,2}^{(1,0;c)}(E_u) = -\frac{\sqrt{14}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{14}$

$\boxed{\text{z505}}$ $\mathbb{Q}_{3,1}^{(1,0;c)}(E_u,1) = -\frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{28} + \frac{3\sqrt{14}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{28} - \frac{\sqrt{14}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{7}$

$\boxed{\text{z506}}$ $\mathbb{Q}_{3,2}^{(1,0;c)}(E_u,1) = -\frac{\sqrt{42}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{28} - \frac{3\sqrt{14}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{28} - \frac{\sqrt{14}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{7}$

$\boxed{\text{z507}}$ $\mathbb{Q}_{3,1}^{(1,0;c)}(E_u,2) = -\frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$

$\boxed{\text{z508}}$ $\mathbb{Q}_{3,2}^{(1,0;c)}(E_u,2) = -\frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$

$\boxed{\text{z509}}$ $\mathbb{Q}_{1,1}^{(1,1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z510}}$ $\mathbb{Q}_{1,2}^{(1,1;c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z511}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{110}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{22} + \frac{\sqrt{66}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{22} - \frac{\sqrt{66}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{22}$

$\boxed{\text{z512}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{110}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{22} - \frac{\sqrt{66}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{22} - \frac{\sqrt{66}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{22}$

- 'A'-'A' bond-cluster : `A;A_003_1`
  - * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  - * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  - * wyckoff: `1a@1b`

$\boxed{\text{z26}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z291}}$ $\mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z513}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z514}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

- 'A'-'A' bond-cluster : `A;A_003_1`
  - * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  - * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
  - * wyckoff: `1a@1b`

$\boxed{\text{z27}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{T}_1^{(a)}(A_{2u})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z28}}$ $\mathbb{Q}_0^{(1,0;c)}(A_{1g}) = \mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z62}}$ $\mathbb{G}_2^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z63}}$ $\mathbb{G}_0^{(1,1;c)}(A_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z95}}$ $\mathbb{G}_1^{(1,-1;c)}(A_{2g}) = \mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z132}}$ $\mathbb{G}_1^{(1,1;c)}(A_{2g}) = \mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z201}}$ $\mathbb{Q}_1^{(c)}(A_{2u}) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z202}}$ $\mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z203}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z204}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z205}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = -\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z206}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z292}}$ $\mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z293}}$ $\mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z340}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z341}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z380}}$ $\mathbb{Q}_{2,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z424}}$ $\mathbb{Q}_{2,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z515}}$ $\mathbb{Q}_{1,1}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z516}}$ $\mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z517}}$ $\mathbb{Q}_{1,1}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z518}}$ $\mathbb{Q}_{1,2}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z519}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = \dfrac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z520}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = \dfrac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

- 'A'-'A' bond-cluster : `A;A_003_1`
  * bra: $\langle p_x,\uparrow|$, $\langle p_x,\downarrow|$, $\langle p_y,\uparrow|$, $\langle p_y,\downarrow|$, $\langle p_z,\uparrow|$, $\langle p_z,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
  * wyckoff: `1a@1b`

$\boxed{\text{z29}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z30}}$ $\mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z31}}$ $\mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z32}}$ $\mathbb{Q}_0^{(1,1;c)}(A_{1g}) = \mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z64}}$ $\mathbb{G}_0^{(c)}(A_{1u}) = \mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z96}}$ $\mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z97}}$ $\mathbb{G}_2^{(1,-1;c)}(A_{1u}) = \mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z133}}$ $\mathbb{G}_0^{(1,1;c)}(A_{1u}) = \mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z134}}$ $\mathbb{G}_1^{(1,0;c)}(A_{2g}) = \mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z207}}$ $\mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z208}}$ $\mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z209}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z210}}$ $\mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = -\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z211}}$ $\mathbb{Q}_3^{(1,0;c)}(B_{1u}) = \mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z212}}$ $\mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z294}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z295}}$ $\mathbb{Q}_3^{(1,-1;c)}(B_{2u}) = \mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z296}}$ $\mathbb{Q}_3^{(1,0;c)}(B_{2u}) = \mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z297}}$ $\mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z342}}$ $\mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z381}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z382}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z425}}$ $\mathbb{G}_{1,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z426}}$ $\mathbb{G}_{1,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z521}}$ $\mathbb{Q}_{1,1}^{(c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z522}}$ $\mathbb{Q}_{1,2}^{(c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z523}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z524}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z525}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,1) = \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{4}$

$\boxed{\text{z526}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,1) = \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{4}$

$\boxed{\text{z527}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,2) = -\frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{4}$

$\boxed{\text{z528}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,2) = -\frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{4}$

$\boxed{\text{z529}}$ $\mathbb{Q}_{1,1}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z530}}$ $\mathbb{Q}_{1,2}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z531}}$ $\mathbb{Q}_{1,1}^{(1,1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z532}}$ $\mathbb{Q}_{1,2}^{(1,1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

- 'A'-'A' bond-cluster : `A;A_004_1`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: `4e@2e`

$\boxed{\text{z33}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z98}}$ $\mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$

$\boxed{\text{z213}}$ $\mathbb{G}_2^{(1,-1;c)}(A_{1u}) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$

$\boxed{\text{z214}}$ $\mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z298}}$ $\mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z299}}$ $\mathbb{Q}_{3}^{(1,-1;c)}(B_{1u}) = \mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{M}_{2}^{(b)}(B_{2u})$

$\boxed{\text{z343}}$ $\mathbb{G}_{2}^{(1,-1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z383}}$ $\mathbb{G}_{2}^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z384}}$ $\mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z427}}$ $\mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z533}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u,a) = -\frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1}^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z534}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u,a) = -\frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1}^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z535}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u,b) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{M}_{2}^{(b)}(B_{2u})}{2}$

$\boxed{\text{z536}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u,b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{M}_{2}^{(b)}(B_{2u})}{2}$

$\boxed{\text{z537}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = -\frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1}^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z538}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = -\frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1}^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

- 'A'-'A' bond-cluster : `A;A_004_1`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
  * wyckoff: `4e@2e`

$\boxed{\text{z34}}$ $\mathbb{Q}_{0}^{(c)}(A_{1g}) = \frac{\sqrt{3}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{T}_{1}^{(a)}(A_{2u})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$

$\boxed{\text{z35}}$ $\mathbb{Q}_2^{(c)}(A_{1g}) = -\frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{T}_{1}^{(a)}(A_{2u})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$

$\boxed{\text{z36}}$ $\mathbb{Q}_0^{(1,-1;c)}(A_{1g}) = \mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{M}_2^{(b)}(B_{2u})$

$\boxed{\text{z37}}$ $\mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z38}}$ $\mathbb{Q}_0^{(1,0;c)}(A_{1g}) = \frac{\sqrt{3}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{T}_{1}^{(1,0;a)}(A_{2u})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$

$\boxed{\text{z39}}$ $\mathbb{Q}_2^{(1,0;c)}(A_{1g}) = -\frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{T}_{1}^{(1,0;a)}(A_{2u})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$

$\boxed{\text{z65}}$ $\mathbb{G}_2^{(c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z66}}$ $\mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_{2}^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2}^{(b)}(B_{1g})}{3}$

$\boxed{\text{z67}}$ $\mathbb{G}_2^{(1,-1;c)}(A_{1u}, a) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z68}}$ $\mathbb{G}_2^{(1,-1;c)}(A_{1u}, b) = \frac{\sqrt{6}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{2}^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2}^{(b)}(B_{1g})}{3}$

$\boxed{\text{z69}}$ $\mathbb{G}_2^{(1,0;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z70}}$ $\mathbb{G}_0^{(1,1;c)}(A_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z99}}$ $\mathbb{Q}_4^{(1,-1;c)}(A_{2g}) = \mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{M}_2^{(b)}(B_{2u})$

$\boxed{\text{z100}}$ $\mathbb{G}_1^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z101}}$ $\mathbb{G}_1^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{30}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{M}_{2}^{(1,-1;a)}(A_{1u})\mathbb{T}_{1}^{(b)}(A_{2u})}{5}$

$\boxed{\text{z102}}$ $\mathbb{G}_3^{(1,-1;c)}(A_{2g}) = -\frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{5} + \frac{\sqrt{5}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{M}_{2}^{(1,-1;a)}(A_{1u})\mathbb{T}_{1}^{(b)}(A_{2u})}{5}$

$\boxed{\text{z103}}$ $$\mathbb{G}_1^{(1,0;c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$\boxed{\text{z104}}$ $$\mathbb{G}_1^{(1,1;c)}(A_{2g}) = \mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_1^{(b)}(A_{2u})$$

$\boxed{\text{z135}}$ $$\mathbb{Q}_1^{(c)}(A_{2u}, a) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$\boxed{\text{z136}}$ $$\mathbb{Q}_1^{(c)}(A_{2u}, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$\boxed{\text{z137}}$ $$\mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$\boxed{\text{z138}}$ $$\mathbb{Q}_3^{(1,-1;c)}(A_{2u}) = -\frac{\sqrt{3}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$\boxed{\text{z139}}$ $$\mathbb{Q}_1^{(1,0;c)}(A_{2u}, a) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$\boxed{\text{z140}}$ $$\mathbb{Q}_1^{(1,0;c)}(A_{2u}, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$\boxed{\text{z215}}$ $$\mathbb{Q}_2^{(c)}(B_{1g}, a) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z216}}$ $$\mathbb{Q}_2^{(c)}(B_{1g}, b) = -\mathbb{T}_1^{(a)}(A_{2u})\mathbb{M}_2^{(b)}(B_{2u})$$

$\boxed{\text{z217}}$ $$\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = -\frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$\boxed{\text{z218}}$ $$\mathbb{Q}_2^{(1,0;c)}(B_{1g}, a) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z219}}$ $$\mathbb{Q}_2^{(1,0;c)}(B_{1g}, b) = -\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{M}_2^{(b)}(B_{2u})$$

$\boxed{\text{z220}}$ $$\mathbb{G}_3^{(1,-1;c)}(B_{1g}) = \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$\boxed{\text{z221}}$ $$\mathbb{Q}_3^{(c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$\boxed{\text{z222}}$ $\mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z223}}$ $\mathbb{Q}_3^{(1,0;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z224}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u}, a) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z225}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u}, b) = -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z226}}$ $\mathbb{G}_2^{(1,1;c)}(B_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z227}}$ $\mathbb{Q}_2^{(c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z228}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}, a) = -\frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$

$\boxed{\text{z229}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}, b) = -\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{M}_2^{(b)}(B_{2u})$

$\boxed{\text{z230}}$ $\mathbb{Q}_2^{(1,0;c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z231}}$ $\mathbb{Q}_2^{(1,1;c)}(B_{2g}) = \mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{M}_2^{(b)}(B_{2u})$

$\boxed{\text{z232}}$ $\mathbb{G}_3^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$

$\boxed{\text{z233}}$ $\mathbb{Q}_3^{(c)}(B_{2u}) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$

$\boxed{\text{z234}}$ $\mathbb{Q}_3^{(1,0;c)}(B_{2u}) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$

$\boxed{\text{z235}}$ $\mathbb{G}_2^{(c)}(B_{2u}) = -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$

$\boxed{\text{z236}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{2u}, a) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$

$$\boxed{\text{z237}} \quad \mathbb{G}_{2}^{(1,-1;c)}(B_{2u},b) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z238}} \quad \mathbb{G}_{2}^{(1,0;c)}(B_{2u}) = -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_{1}^{(1,0;a)}(A_{2u})\mathbb{Q}_{2}^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z300}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g,a) = \frac{\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1}^{(b)}(A_{2u})}{2} + \frac{\mathbb{T}_{1}^{(a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z301}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g,a) = \frac{\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1}^{(b)}(A_{2u})}{2} + \frac{\mathbb{T}_{1}^{(a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z302}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g,b) = -\frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{M}_{2}^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z303}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g,b) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{M}_{2}^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z304}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g,a) = \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1}^{(b)}(A_{2u})}{6} + \frac{\mathbb{M}_{2}^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{M}_{2}^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{3}\mathbb{M}_{2}^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z305}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g,a) = \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1}^{(b)}(A_{2u})}{6} - \frac{\mathbb{M}_{2}^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{M}_{2}^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{3}\mathbb{M}_{2}^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z344}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g,b) = -\frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_{2}^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z345}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g,b) = \frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_{2}^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z346}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g,a) = \frac{\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_{1}^{(b)}(A_{2u})}{2} + \frac{\mathbb{T}_{1}^{(1,0;a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z347}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g,a) = \frac{\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_{1}^{(b)}(A_{2u})}{2} + \frac{\mathbb{T}_{1}^{(1,0;a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z348}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g,b) = -\frac{\sqrt{2}\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{M}_{2}^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z349}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g,b) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{M}_{2}^{(b)}(B_{2u})}{2}$$

$\boxed{\text{z385}}$ $$\mathbb{G}_{1,1}^{(c)}(E_g) = \frac{\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{T}_1^{(a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z386}}$ $$\mathbb{G}_{1,2}^{(c)}(E_g) = \frac{\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{T}_1^{(a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$\boxed{\text{z387}}$ $$\mathbb{G}_{1,1}^{(1,-1;c)}(E_g) = -\frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$$

$\boxed{\text{z388}}$ $$\mathbb{G}_{1,2}^{(1,-1;c)}(E_g) = -\frac{\sqrt{15}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$$

$\boxed{\text{z389}}$ $$\mathbb{G}_{3,1}^{(1,-1;c)}(E_g,1) = \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{20} - \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$$

$\boxed{\text{z390}}$ $$\mathbb{G}_{3,2}^{(1,-1;c)}(E_g,1) = \frac{\sqrt{10}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{20} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$$

$\boxed{\text{z428}}$ $$\mathbb{G}_{3,1}^{(1,-1;c)}(E_g,2) = \frac{\sqrt{6}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{6} - \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{6}$$

$\boxed{\text{z429}}$ $$\mathbb{G}_{3,2}^{(1,-1;c)}(E_g,2) = \frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{6} + \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{12} - \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{6}$$

$\boxed{\text{z430}}$ $$\mathbb{G}_{1,1}^{(1,0;c)}(E_g) = \frac{\mathbb{T}_{1,2}^{(1,0;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z431}}$ $$\mathbb{G}_{1,2}^{(1,0;c)}(E_g) = \frac{\mathbb{T}_{1,1}^{(1,0;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$\boxed{\text{z432}}$ $$\mathbb{G}_{1,1}^{(1,1;c)}(E_g) = \frac{\sqrt{2}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$\boxed{\text{z433}}$ $$\mathbb{G}_{1,2}^{(1,1;c)}(E_g) = -\frac{\sqrt{2}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z539}}$ $$\mathbb{Q}_{1,1}^{(c)}(E_u,a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z540}}$ $$\mathbb{Q}_{1,2}^{(c)}(E_u,a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z541}}$ $\mathbb{Q}_{1,1}^{(c)}(E_u,b)=\frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}+\frac{\mathbb{Q}_{1}^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z542}}$ $\mathbb{Q}_{1,2}^{(c)}(E_u,b)=-\frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}+\frac{\mathbb{Q}_{1}^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z543}}$ $\mathbb{Q}_{3,1}^{(c)}(E_u,1)=\frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}-\frac{\mathbb{Q}_{1}^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z544}}$ $\mathbb{Q}_{3,2}^{(c)}(E_u,1)=-\frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}-\frac{\mathbb{Q}_{1}^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z545}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u)=\frac{\sqrt{3}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{6}-\frac{\mathbb{G}_{2}^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}-\frac{\sqrt{3}\mathbb{G}_{2}^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6}+\frac{\sqrt{3}\mathbb{G}_{2}^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$

$\boxed{\text{z546}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u)=-\frac{\sqrt{3}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{6}+\frac{\mathbb{G}_{2}^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}-\frac{\sqrt{3}\mathbb{G}_{2}^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}-\frac{\sqrt{3}\mathbb{G}_{2}^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6}$

$\boxed{\text{z547}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,1)=-\frac{\sqrt{15}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{30}+\frac{\sqrt{5}\mathbb{G}_{2}^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}+\frac{\sqrt{15}\mathbb{G}_{2}^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30}+\frac{\sqrt{15}\mathbb{G}_{2}^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$

$\boxed{\text{z548}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,1)=\frac{\sqrt{15}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{30}-\frac{\sqrt{5}\mathbb{G}_{2}^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}+\frac{\sqrt{15}\mathbb{G}_{2}^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30}-\frac{\sqrt{15}\mathbb{G}_{2}^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6}$

$\boxed{\text{z549}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,2)=\frac{\sqrt{15}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{10}+\frac{\sqrt{5}\mathbb{G}_{2}^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5}-\frac{\sqrt{15}\mathbb{G}_{2}^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}$

$\boxed{\text{z550}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,2)=-\frac{\sqrt{15}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{10}-\frac{\sqrt{5}\mathbb{G}_{2}^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{5}-\frac{\sqrt{15}\mathbb{G}_{2}^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}$

$\boxed{\text{z551}}$ $\mathbb{Q}_{1,1}^{(1,0;c)}(E_u,a)=\frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z552}}$ $\mathbb{Q}_{1,2}^{(1,0;c)}(E_u,a)=\frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z553}}$ $\mathbb{Q}_{1,1}^{(1,0;c)}(E_u,b)=\frac{\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}+\frac{\mathbb{Q}_{1}^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z554}}$ $\mathbb{Q}_{1,2}^{(1,0;c)}(E_u,b)=-\frac{\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}+\frac{\mathbb{Q}_{1}^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z555}}$ $\mathbb{Q}_{3,1}^{(1,0;c)}(E_u,1) = \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_{1}^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z556}}$ $\mathbb{Q}_{3,2}^{(1,0;c)}(E_u,1) = -\frac{\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_{1}^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z557}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E_u,a) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z558}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E_u,a) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z559}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E_u,b) = -\frac{\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_{2}^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z560}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E_u,b) = \frac{\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_{2}^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z561}}$ $\mathbb{G}_{2,1}^{(1,1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{0}^{(1,1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z562}}$ $\mathbb{G}_{2,2}^{(1,1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{G}_{0}^{(1,1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

- 'A'-'A' bond-cluster : `A;A_004_1`
  - * bra: $\langle p_x,\uparrow|$, $\langle p_x,\downarrow|$, $\langle p_y,\uparrow|$, $\langle p_y,\downarrow|$, $\langle p_z,\uparrow|$, $\langle p_z,\downarrow|$
  - * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
  - * wyckoff: `4e@2e`

$\boxed{\text{z40}}$ $\mathbb{Q}_{0}^{(c)}(A_{1g},a) = \mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{0}^{(b)}(A_{1g})$

$\boxed{\text{z41}}$ $\mathbb{Q}_{0}^{(c)}(A_{1g},b) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_{2}^{(a)}(B_{1g})\mathbb{Q}_{2}^{(b)}(B_{1g})}{3}$

$\boxed{\text{z42}}$ $\mathbb{Q}_{2}^{(c)}(A_{1g},a) = \mathbb{Q}_{2}^{(a)}(A_{1g})\mathbb{Q}_{0}^{(b)}(A_{1g})$

$\boxed{\text{z43}}$ $\mathbb{Q}_{2}^{(c)}(A_{1g},b) = \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{Q}_{2}^{(a)}(B_{1g})\mathbb{Q}_{2}^{(b)}(B_{1g})}{3}$

$\boxed{\text{z44}}$ $$\mathbb{Q}_0^{(1,-1;c)}(A_{1g}) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_{2}^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2}^{(b)}(B_{1g})}{3}$$

$\boxed{\text{z45}}$ $$\mathbb{Q}_2^{(1,-1;c)}(A_{1g},a) = \mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$\boxed{\text{z46}}$ $$\mathbb{Q}_2^{(1,-1;c)}(A_{1g},b) = \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{Q}_{2}^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2}^{(b)}(B_{1g})}{3}$$

$\boxed{\text{z47}}$ $$\mathbb{Q}_2^{(1,0;c)}(A_{1g}) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$\boxed{\text{z48}}$ $$\mathbb{Q}_0^{(1,1;c)}(A_{1g}) = \mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$\boxed{\text{z71}}$ $$\mathbb{Q}_5^{(1,-1;c)}(A_{1u}) = \mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{M}_2^{(b)}(B_{2u})$$

$\boxed{\text{z72}}$ $$\mathbb{G}_0^{(c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_{1}^{(a)}(A_{2g})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$$

$\boxed{\text{z73}}$ $$\mathbb{G}_2^{(c)}(A_{1u}) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{1}^{(a)}(A_{2g})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$$

$\boxed{\text{z74}}$ $$\mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$$

$\boxed{\text{z75}}$ $$\mathbb{G}_2^{(1,-1;c)}(A_{1u},a) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$$

$\boxed{\text{z76}}$ $$\mathbb{G}_2^{(1,-1;c)}(A_{1u},b) = -\frac{\sqrt{21}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{35}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{35}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{M}_{3}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1}^{(b)}(A_{2u})}{7}$$

$\boxed{\text{z105}}$ $$\mathbb{G}_4^{(1,-1;c)}(A_{1u},1) = \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_{3}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$$

$\boxed{\text{z106}}$ $$\begin{aligned}\mathbb{G}_4^{(1,-1;c)}(A_{1u},2) = &-\frac{\sqrt{105}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{42} + \frac{3\sqrt{7}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{105}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{42}\\ &- \frac{3\sqrt{7}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{105}\mathbb{M}_{3}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1}^{(b)}(A_{2u})}{21}\end{aligned}$$

$\boxed{\text{z107}}$ $$\mathbb{G}_0^{(1,0;c)}(A_{1u}) = \mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{M}_2^{(b)}(B_{2u})$$

$\boxed{\text{z108}}$ $$\mathbb{G}_2^{(1,0;c)}(A_{1u}) = -\frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z109}}$ $$\mathbb{G}_0^{(1,1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_{1}^{(1,1;a)}(A_{2g})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$$

$\boxed{\text{z110}}$ $$\mathbb{G}_2^{(1,1;c)}(A_{1u}) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{1}^{(1,1;a)}(A_{2g})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$$

$\boxed{\text{z111}}$ $$\mathbb{Q}_4^{(c)}(A_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$\boxed{\text{z112}}$ $$\mathbb{Q}_4^{(1,-1;c)}(A_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$\boxed{\text{z113}}$ $$\mathbb{G}_1^{(c)}(A_{2g}) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$\boxed{\text{z141}}$ $$\mathbb{G}_1^{(1,-1;c)}(A_{2g}) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$\boxed{\text{z142}}$ $$\mathbb{G}_1^{(1,0;c)}(A_{2g},a) = \mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$\boxed{\text{z143}}$ $$\mathbb{G}_1^{(1,0;c)}(A_{2g},b) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$\boxed{\text{z144}}$ $$\mathbb{Q}_1^{(c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$\boxed{\text{z145}}$ $$\mathbb{Q}_1^{(1,-1;c)}(A_{2u},a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$\boxed{\text{z146}}$ $$\mathbb{Q}_1^{(1,-1;c)}(A_{2u},b) = \mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{M}_2^{(b)}(B_{2u})$$

$\boxed{\text{z239}}$ $$\mathbb{Q}_3^{(1,-1;c)}(A_{2u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$$

$\boxed{\text{z240}}$ $$\mathbb{Q}_1^{(1,0;c)}(A_{2u},a) = \frac{\sqrt{30}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{10} + \frac{\sqrt{30}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{T}_{2}^{(1,0;a)}(A_{1g})\mathbb{T}_{1}^{(b)}(A_{2u})}{5}$$

$\boxed{\text{z241}}$ $$\mathbb{Q}_1^{(1,0;c)}(A_{2u},b) = \mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{M}_2^{(b)}(B_{2u})$$

$\boxed{\text{z242}}$ $\mathbb{Q}_3^{(1,0;c)}(A_{2u}) = -\frac{\sqrt{5}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{5} - \frac{\sqrt{5}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{T}_{2}^{(1,0;a)}(A_{1g})\mathbb{T}_{1}^{(b)}(A_{2u})}{5}$

$\boxed{\text{z243}}$ $\mathbb{Q}_1^{(1,1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z244}}$ $\mathbb{G}_4^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$

$\boxed{\text{z245}}$ $\mathbb{Q}_2^{(c)}(B_{1g},a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z246}}$ $\mathbb{Q}_2^{(c)}(B_{1g},b) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z247}}$ $\mathbb{Q}_2^{(c)}(B_{1g},c) = -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{10}\mathbb{Q}_{2}^{(a)}(A_{1g})\mathbb{Q}_{2}^{(b)}(B_{1g})}{5}$

$\boxed{\text{z248}}$ $\mathbb{Q}_4^{(c)}(B_{1g}) = \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} - \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} - \frac{\sqrt{15}\mathbb{Q}_{2}^{(a)}(A_{1g})\mathbb{Q}_{2}^{(b)}(B_{1g})}{5}$

$\boxed{\text{z249}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{1g},a) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z250}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{1g},b) = -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{10}\mathbb{Q}_{2}^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2}^{(b)}(B_{1g})}{5}$

$\boxed{\text{z251}}$ $\mathbb{Q}_4^{(1,-1;c)}(B_{1g}) = \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} - \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} - \frac{\sqrt{15}\mathbb{Q}_{2}^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2}^{(b)}(B_{1g})}{5}$

$\boxed{\text{z252}}$ $\mathbb{Q}_2^{(1,0;c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z253}}$ $\mathbb{Q}_2^{(1,1;c)}(B_{1g}) = \mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z254}}$ $\mathbb{Q}_3^{(c)}(B_{1u}) = \mathbb{M}_1^{(a)}(A_{2g})\mathbb{M}_2^{(b)}(B_{2u})$

$\boxed{\text{z255}}$ $\mathbb{Q}_3^{(1,-1;c)}(B_{1u},a) = \mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{M}_2^{(b)}(B_{2u})$

$\boxed{\text{z256}}$ $\mathbb{Q}_3^{(1,-1;c)}(B_{1u},b) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$

$\boxed{\text{z257}}$ $\mathbb{Q}_3^{(1,-1;c)}(B_{1u},c) = -\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{M}_2^{(b)}(B_{2u})$

$\boxed{\text{z258}}$ $\mathbb{Q}_3^{(1,0;c)}(B_{1u}) = \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$

$\boxed{\text{z259}}$ $\mathbb{Q}_3^{(1,1;c)}(B_{1u}) = \mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{M}_2^{(b)}(B_{2u})$

$\boxed{\text{z260}}$ $\mathbb{G}_2^{(c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z261}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u},a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z262}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u},b) = \frac{3\sqrt{7}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{105}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{42} + \frac{3\sqrt{7}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{14}$
$- \frac{\sqrt{105}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{42} + \frac{\sqrt{105}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{21}$

$\boxed{\text{z263}}$ $\mathbb{G}_4^{(1,-1;c)}(B_{1u}) = \frac{\sqrt{35}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{35}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{7}$

$\boxed{\text{z264}}$ $\mathbb{G}_2^{(1,0;c)}(B_{1u}) = -\frac{\sqrt{6}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$

$\boxed{\text{z265}}$ $\mathbb{G}_2^{(1,1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z266}}$ $\mathbb{Q}_2^{(c)}(B_{2g},a) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z267}}$ $\mathbb{Q}_2^{(c)}(B_{2g},b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z268}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{2g},a) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z306}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{2g},b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z307}}$ $\mathbb{Q}_2^{(1,0;c)}(B_{2g}) = -\frac{\sqrt{6}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{G}_1^{(1,0;a)}(A_{2g})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$

$\boxed{\text{z308}}$ $\mathbb{G}_{3}^{(1,0;c)}(B_{2g}) = \frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_{1}^{(1,0;a)}(A_{2g})\mathbb{Q}_{2}^{(b)}(B_{1g})}{3}$

$\boxed{\text{z309}}$ $\mathbb{Q}_{3}^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{12} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{3}\mathbb{M}_{3}^{(1,-1;a)}(B_{1g})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$

$\boxed{\text{z310}}$ $\mathbb{Q}_{3}^{(1,0;c)}(B_{2u},a) = -\frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{T}_{2}^{(1,0;a)}(B_{1g})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$

$\boxed{\text{z311}}$ $\mathbb{Q}_{3}^{(1,0;c)}(B_{2u},b) = -\mathbb{T}_{2}^{(1,0;a)}(A_{1g})\mathbb{M}_{2}^{(b)}(B_{2u})$

$\boxed{\text{z312}}$ $\mathbb{G}_{2}^{(c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z313}}$ $\mathbb{G}_{2}^{(1,-1;c)}(B_{2u},a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z314}}$ $\mathbb{G}_{2}^{(1,-1;c)}(B_{2u},b) = -\frac{\sqrt{7}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{7} + \frac{\sqrt{105}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{21} + \frac{\sqrt{7}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{7} - \frac{\sqrt{105}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{21} + \frac{\sqrt{105}\mathbb{M}_{3}^{(1,-1;a)}(B_{1g})\mathbb{T}_{1}^{(b)}(A_{2u})}{21}$

$\boxed{\text{z315}}$ $\mathbb{G}_{4}^{(1,-1;c)}(B_{2u}) = -\frac{\sqrt{35}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{28} - \frac{3\sqrt{21}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{28} + \frac{\sqrt{35}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{28} + \frac{3\sqrt{21}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{28} + \frac{\sqrt{21}\mathbb{M}_{3}^{(1,-1;a)}(B_{1g})\mathbb{T}_{1}^{(b)}(A_{2u})}{7}$

$\boxed{\text{z316}}$ $\mathbb{G}_{2}^{(1,0;c)}(B_{2u}) = -\frac{\sqrt{6}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{T}_{2}^{(1,0;a)}(B_{1g})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$

$\boxed{\text{z317}}$ $\mathbb{G}_{2}^{(1,1;c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z350}}$ $\mathbb{Q}_{2,1}^{(c)}(E_g,a) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z351}}$ $\mathbb{Q}_{2,2}^{(c)}(E_g,a) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z352}}$ $\mathbb{Q}_{2,1}^{(c)}(E_g,b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z353}}$ $$\mathbb{Q}_{2,2}^{(c)}(E_g,b)=\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z354}}$ $$\mathbb{Q}_{2,1}^{(c)}(E_g,c)=-\frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{10}+\frac{\sqrt{5}\mathbb{Q}_{2}^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}-\frac{\sqrt{15}\mathbb{Q}_{2}^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}+\frac{\sqrt{15}\mathbb{Q}_{2}^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}$$

$\boxed{\text{z355}}$ $$\mathbb{Q}_{2,2}^{(c)}(E_g,c)=\frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{10}+\frac{\sqrt{5}\mathbb{Q}_{2}^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}+\frac{\sqrt{15}\mathbb{Q}_{2}^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}+\frac{\sqrt{15}\mathbb{Q}_{2}^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}$$

$\boxed{\text{z356}}$ $$\mathbb{Q}_{4,1}^{(c)}(E_g,1)=-\frac{7\sqrt{235}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{470}-\frac{11\sqrt{705}\mathbb{Q}_{2}^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{470}-\frac{7\sqrt{235}\mathbb{Q}_{2}^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{470}-\frac{3\sqrt{235}\mathbb{Q}_{2}^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{470}$$

$\boxed{\text{z357}}$ $$\mathbb{Q}_{4,2}^{(c)}(E_g,1)=\frac{7\sqrt{235}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{470}-\frac{11\sqrt{705}\mathbb{Q}_{2}^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{470}+\frac{7\sqrt{235}\mathbb{Q}_{2}^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{470}-\frac{3\sqrt{235}\mathbb{Q}_{2}^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{470}$$

$\boxed{\text{z358}}$ $$\mathbb{Q}_{4,1}^{(c)}(E_g,2)=\frac{3\sqrt{47}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{94}-\frac{\sqrt{141}\mathbb{Q}_{2}^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{47}+\frac{3\sqrt{47}\mathbb{Q}_{2}^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{94}+\frac{4\sqrt{47}\mathbb{Q}_{2}^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{47}$$

$\boxed{\text{z391}}$ $$\mathbb{Q}_{4,2}^{(c)}(E_g,2)=-\frac{3\sqrt{47}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{94}-\frac{\sqrt{141}\mathbb{Q}_{2}^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{47}-\frac{3\sqrt{47}\mathbb{Q}_{2}^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{94}+\frac{4\sqrt{47}\mathbb{Q}_{2}^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{47}$$

$\boxed{\text{z392}}$ $$\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g,a)=\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z393}}$ $$\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g,a)=\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z394}}$ $$\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g,b)=-\frac{\sqrt{15}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{10}+\frac{\sqrt{5}\mathbb{Q}_{2}^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}-\frac{\sqrt{15}\mathbb{Q}_{2}^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}+\frac{\sqrt{15}\mathbb{Q}_{2}^{(1,-1;a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}$$

$\boxed{\text{z395}}$ $$\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g,b)=\frac{\sqrt{15}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{10}+\frac{\sqrt{5}\mathbb{Q}_{2}^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}+\frac{\sqrt{15}\mathbb{Q}_{2}^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}+\frac{\sqrt{15}\mathbb{Q}_{2}^{(1,-1;a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}$$

$\boxed{\text{z396}}$ $$\mathbb{Q}_{4,1}^{(1,-1;c)}(E_g,1)=-\frac{7\sqrt{235}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{470}-\frac{11\sqrt{705}\mathbb{Q}_{2}^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{470}-\frac{7\sqrt{235}\mathbb{Q}_{2}^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{470}-\frac{3\sqrt{235}\mathbb{Q}_{2}^{(1,-1;a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{470}$$

$\boxed{\text{z397}}$ $$\mathbb{Q}_{4,2}^{(1,-1;c)}(E_g,1)=\frac{7\sqrt{235}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{470}-\frac{11\sqrt{705}\mathbb{Q}_{2}^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{470}+\frac{7\sqrt{235}\mathbb{Q}_{2}^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{470}-\frac{3\sqrt{235}\mathbb{Q}_{2}^{(1,-1;a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{470}$$

$\boxed{\text{z398}}$ $$\mathbb{Q}_{4,1}^{(1,-1;c)}(E_g,2)=\frac{3\sqrt{47}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{94}-\frac{\sqrt{141}\mathbb{Q}_{2}^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{47}+\frac{3\sqrt{47}\mathbb{Q}_{2}^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{94}+\frac{4\sqrt{47}\mathbb{Q}_{2}^{(1,-1;a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{47}$$

$\boxed{\text{z399}}$ $$\mathbb{Q}_{4,2}^{(1,-1;c)}(E_g,2) = -\frac{3\sqrt{47}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{94} - \frac{\sqrt{141}\mathbb{Q}_{2}^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{47} - \frac{3\sqrt{47}\mathbb{Q}_{2}^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{94} + \frac{4\sqrt{47}\mathbb{Q}_{2}^{(1,-1;a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{47}$$

$\boxed{\text{z400}}$ $$\mathbb{Q}_{2,1}^{(1,0;c)}(E_g) = -\frac{\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2} + \frac{\mathbb{G}_{1}^{(1,0;a)}(A_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$\boxed{\text{z401}}$ $$\mathbb{Q}_{2,2}^{(1,0;c)}(E_g) = \frac{\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_{1}^{(1,0;a)}(A_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$\boxed{\text{z402}}$ $$\mathbb{Q}_{2,1}^{(1,1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(1,1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$\boxed{\text{z434}}$ $$\mathbb{Q}_{2,2}^{(1,1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(1,1;a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$\boxed{\text{z435}}$ $$\mathbb{G}_{1,1}^{(c)}(E_g) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_{2}^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$\boxed{\text{z436}}$ $$\mathbb{G}_{1,2}^{(c)}(E_g) = -\frac{\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_{2}^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$\boxed{\text{z437}}$ $$\mathbb{G}_{1,1}^{(1,-1;c)}(E_g) = \frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_{2}^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$\boxed{\text{z438}}$ $$\mathbb{G}_{1,2}^{(1,-1;c)}(E_g) = -\frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_{2}^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$\boxed{\text{z439}}$ $$\mathbb{G}_{1,1}^{(1,0;c)}(E_g,a) = \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z440}}$ $$\mathbb{G}_{1,2}^{(1,0;c)}(E_g,a) = \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z441}}$ $$\mathbb{G}_{1,1}^{(1,0;c)}(E_g,b) = \frac{\mathbb{G}_{1,1}^{(1,0;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2} + \frac{\mathbb{G}_{1}^{(1,0;a)}(A_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$\boxed{\text{z442}}$ $$\mathbb{G}_{1,2}^{(1,0;c)}(E_g,b) = -\frac{\mathbb{G}_{1,2}^{(1,0;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_{1}^{(1,0;a)}(A_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$\boxed{\text{z563}}$ $$\mathbb{Q}_{1,1}^{(c)}(E_u,a) = -\frac{\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_{1}^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_{1}^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z564}}$ $\mathbb{Q}_{1,2}^{(c)}(E_u,a) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z565}}$ $\mathbb{Q}_{1,1}^{(c)}(E_u,b) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$

$\boxed{\text{z566}}$ $\mathbb{Q}_{1,2}^{(c)}(E_u,b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$

$\boxed{\text{z567}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u,a) = -\frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z568}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u,a) = -\frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z569}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u,b) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$

$\boxed{\text{z570}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u,b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$

$\boxed{\text{z571}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u,c) = \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{M}_2^{(b)}(B_{2u})}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{M}_2^{(b)}(B_{2u})}{4}$

$\boxed{\text{z572}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u,c) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{M}_2^{(b)}(B_{2u})}{4} + \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{M}_2^{(b)}(B_{2u})}{4}$

$\boxed{\text{z573}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,1) = \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{8}$

$\boxed{\text{z574}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,1) = \frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$

$\boxed{\text{z575}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,2a) = -\frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{24} + \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{24}$

$\boxed{\text{z576}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,2a) = -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{24} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{24}$

$\boxed{\text{z577}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,2b) = -\frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{M}_2^{(b)}(B_{2u})}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{M}_2^{(b)}(B_{2u})}{4}$

$\boxed{\text{z578}}$ $$\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,2b) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{M}_2^{(b)}(B_{2u})}{4} + \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{M}_2^{(b)}(B_{2u})}{4}$$

$\boxed{\text{z579}}$ $$\mathbb{Q}_{1,1}^{(1,0;c)}(E_u,a) = \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{5}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$$

$\boxed{\text{z580}}$ $$\mathbb{Q}_{1,2}^{(1,0;c)}(E_u,a) = \frac{\sqrt{15}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{5}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{15}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$$

$\boxed{\text{z581}}$ $$\mathbb{Q}_{1,1}^{(1,0;c)}(E_u,b) = -\frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$\boxed{\text{z582}}$ $$\mathbb{Q}_{1,2}^{(1,0;c)}(E_u,b) = \frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$\boxed{\text{z583}}$ $$\mathbb{Q}_{3,1}^{(1,0;c)}(E_u,1) = -\frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{30}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{20} - \frac{\sqrt{10}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$$

$\boxed{\text{z584}}$ $$\mathbb{Q}_{3,2}^{(1,0;c)}(E_u,1) = -\frac{\sqrt{10}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{30}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{20} - \frac{3\sqrt{10}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{20} - \frac{\sqrt{10}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$$

$\boxed{\text{z585}}$ $$\mathbb{Q}_{3,1}^{(1,0;c)}(E_u,2) = -\frac{\sqrt{6}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{6} - \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{6}$$

$\boxed{\text{z586}}$ $$\mathbb{Q}_{3,2}^{(1,0;c)}(E_u,2) = -\frac{\sqrt{6}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{6} - \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{12} + \frac{\sqrt{6}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{6}$$

$\boxed{\text{z587}}$ $$\mathbb{Q}_{1,1}^{(1,1;c)}(E_u,a) = -\frac{\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z588}}$ $$\mathbb{Q}_{1,2}^{(1,1;c)}(E_u,a) = -\frac{\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$\boxed{\text{z589}}$ $$\mathbb{Q}_{1,1}^{(1,1;c)}(E_u,b) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$\boxed{\text{z590}}$ $$\mathbb{Q}_{1,2}^{(1,1;c)}(E_u,b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{2u})}{2}$$

$\boxed{\text{z591}}$ $$\mathbb{G}_{2,1}^{(c)}(E_u) = -\frac{\mathbb{M}_{1,2}^{(a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z592}}$ $\mathbb{G}_{2,2}^{(c)}(E_u) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z593}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E_u,a) = -\frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z594}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E_u,a) = -\frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z595}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E_u,b) = \frac{\sqrt{14}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{14} + \frac{\sqrt{210}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{42} - \frac{\sqrt{14}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{210}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{42} - \frac{\sqrt{210}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{42}$

$\boxed{\text{z596}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E_u,b) = \frac{\sqrt{14}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{14} + \frac{\sqrt{210}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{42} + \frac{\sqrt{14}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{210}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{42} - \frac{\sqrt{210}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{42}$

$\boxed{\text{z597}}$ $\mathbb{G}_{4,1}^{(1,-1;c)}(E_u,1) = -\frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{8}$

$\boxed{\text{z598}}$ $\mathbb{G}_{4,2}^{(1,-1;c)}(E_u,1) = -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$

$\boxed{\text{z599}}$ $\mathbb{G}_{4,1}^{(1,-1;c)}(E_u,2) = \frac{\sqrt{70}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{56} - \frac{3\sqrt{42}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{56} - \frac{\sqrt{70}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{56} + \frac{\sqrt{42}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{3\sqrt{42}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{56}$

$\boxed{\text{z600}}$ $\mathbb{G}_{4,2}^{(1,-1;c)}(E_u,2) = \frac{\sqrt{70}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{56} - \frac{3\sqrt{42}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{56} + \frac{\sqrt{70}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{56} - \frac{\sqrt{42}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{14} + \frac{3\sqrt{42}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{56}$

$\boxed{\text{z601}}$ $\mathbb{G}_{2,1}^{(1,0;c)}(E_u) = -\frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{6} + \frac{\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{6}$

$\boxed{\text{z602}}$ $\mathbb{G}_{2,2}^{(1,0;c)}(E_u) = -\frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{6} + \frac{\mathbb{T}_2^{(1,0;a)}(A_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{6}$

$\boxed{\text{z603}}$ $\mathbb{G}_{2,1}^{(1,1;c)}(E_u) = -\frac{\mathbb{M}_{1,2}^{(1,1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z604}}$ $\mathbb{G}_{2,2}^{(1,1;c)}(E_u) = -\frac{\mathbb{M}_{1,1}^{(1,1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(1,1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

- bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
- ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$

$\boxed{\text{x1}}$ $\mathbb{Q}_{0}^{(a)}(A_{1g}) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$

$\boxed{\text{x2}}$ $\mathbb{M}_{1}^{(1,-1;a)}(A_{2g}) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{bmatrix}$

$\boxed{\text{x3}}$ $\mathbb{M}_{1,1}^{(1,-1;a)}(E_{g}) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$

$\boxed{\text{x4}}$ $\mathbb{M}_{1,2}^{(1,-1;a)}(E_{g}) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{2} \\ -\frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$

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

$\boxed{\text{x5}}$ $\mathbb{Q}_{1}^{(a)}(A_{2u}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$

$\boxed{\text{x6}}$ $\mathbb{Q}_{1,1}^{(a)}(E_{u}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x7}}$ $\mathbb{Q}_{1,2}^{(a)}(E_{u}) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$

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

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

$\boxed{\text{x10}}$ $\mathbb{Q}_{1,2}^{(1,0;a)}(E_{u}) = \begin{bmatrix} \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$

$$\boxed{\text{x11}}\quad \mathbb{G}_2^{(1,-1;a)}(A_{1u}) = \begin{bmatrix} 0 & -\frac{\sqrt{6}i}{12} & 0 & -\frac{\sqrt{6}}{12} & \frac{\sqrt{6}i}{6} & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}i}{6} \end{bmatrix}$$

$$\boxed{\text{x12}}\quad \mathbb{G}_2^{(1,-1;a)}(B_{1u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x13}}\quad \mathbb{G}_2^{(1,-1;a)}(B_{2u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x14}}\quad \mathbb{G}_{2,1}^{(1,-1;a)}(E_u) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x15}}\quad \mathbb{G}_{2,2}^{(1,-1;a)}(E_u) = \begin{bmatrix} -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x16}}\quad \mathbb{G}_0^{(1,1;a)}(A_{1u}) = \begin{bmatrix} 0 & \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \end{bmatrix}$$

$$\boxed{\text{x17}}\quad \mathbb{M}_2^{(1,-1;a)}(A_{1u}) = \begin{bmatrix} 0 & -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}}{6} & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{6}}{6} \end{bmatrix}$$

$$\boxed{\text{x18}}\quad \mathbb{M}_2^{(1,-1;a)}(B_{1u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x19}}\quad \mathbb{M}_2^{(1,-1;a)}(B_{2u}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x20}}\quad \mathbb{M}_{2,1}^{(1,-1;a)}(E_u) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x21}}\quad \mathbb{M}_{2,2}^{(1,-1;a)}(E_u) = \begin{bmatrix} -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x22}}\quad \mathbb{M}_0^{(1,1;a)}(A_{1u}) = \begin{bmatrix} 0 & \frac{\sqrt{3}}{6} & 0 & -\frac{\sqrt{3}i}{6} & \frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} \end{bmatrix}$$

$$\boxed{\text{x23}}\quad \mathbb{T}_1^{(a)}(A_{2u}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} \end{bmatrix}$$

$\boxed{\text{x24}}$ $\mathbb{T}_{1,1}^{(a)}(E_u) = \begin{bmatrix} \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x25}}$ $\mathbb{T}_{1,2}^{(a)}(E_u) = \begin{bmatrix} 0 & 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$

$\boxed{\text{x26}}$ $\mathbb{T}_{1}^{(1,0;a)}(A_{2u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x27}}$ $\mathbb{T}_{1,1}^{(1,0;a)}(E_u) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$

$\boxed{\text{x28}}$ $\mathbb{T}_{1,2}^{(1,0;a)}(E_u) = \begin{bmatrix} \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$

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

$\boxed{\text{x29}}$ $\mathbb{Q}_{0}^{(a)}(A_{1g}) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \end{bmatrix}$

$\boxed{\text{x30}}$ $\mathbb{Q}_{2}^{(a)}(A_{1g}) = \begin{bmatrix} -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$

$\boxed{\text{x31}}$ $\mathbb{Q}_{2}^{(a)}(B_{1g}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$

$$\boxed{\text{x32}} \quad \mathbb{Q}_{2}^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x33}} \quad \mathbb{Q}_{2,1}^{(a)}(E_{g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x34}} \quad \mathbb{Q}_{2,2}^{(a)}(E_{g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x35}} \quad \mathbb{Q}_{2}^{(1,-1;a)}(A_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{12} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & \frac{\sqrt{6}i}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x36}} \quad \mathbb{Q}_{2}^{(1,-1;a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x37}} \quad \mathbb{Q}_{2}^{(1,-1;a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x38}}$ $$\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x39}}$ $$\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x40}}$ $$\mathbb{Q}_{0}^{(1,1;a)}(A_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x41}}$ $$\mathbb{G}_{1}^{(1,0;a)}(A_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x42}}$ $$\mathbb{G}_{1,1}^{(1,0;a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x43}}$ $$\mathbb{G}_{1,2}^{(1,0;a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x44}}$ $$\mathbb{M}_{1}^{(a)}(A_{2g}) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x45}}$ $$\mathbb{M}_{1,1}^{(a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x46}}$ $$\mathbb{M}_{1,2}^{(a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x47}}$ $$\mathbb{M}_{1}^{(1,-1;a)}(A_{2g}) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \end{bmatrix}$$

$\boxed{\text{x48}}$ $$\mathbb{M}_{3}^{(1,-1;a)}(A_{2g}) = \begin{bmatrix} -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & \frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{5}}{10} & -\frac{\sqrt{5}i}{10} & 0 \\ 0 & -\frac{\sqrt{5}}{10} & 0 & \frac{\sqrt{5}i}{10} & \frac{\sqrt{5}}{5} & 0 \\ -\frac{\sqrt{5}}{10} & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & -\frac{\sqrt{5}}{5} \end{bmatrix}$$

$\boxed{\text{x49}}$ $$\mathbb{M}_{3}^{(1,-1;a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x50}}$ $$\mathbb{M}_{3}^{(1,-1;a)}(B_{2g}) = \begin{bmatrix} \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x51}}$ $$\mathbb{M}_{1,1}^{(1,-1;a)}(E_{g}) = \begin{bmatrix} 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \end{bmatrix}$$

$\boxed{\text{x52}}$ $$\mathbb{M}_{1,2}^{(1,-1;a)}(E_{g}) = \begin{bmatrix} 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$$

$\boxed{\text{x53}}$ $$\mathbb{M}_{3,1}^{(1,-1;a)}(E_{g},1) = \begin{bmatrix} 0 & \frac{\sqrt{5}}{5} & 0 & \frac{\sqrt{5}i}{10} & -\frac{\sqrt{5}}{10} & 0 \\ \frac{\sqrt{5}}{5} & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & \frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 \\ -\frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 \end{bmatrix}$$

$$\boxed{\text{x54}}\quad \mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)=\begin{bmatrix} 0 & -\frac{\sqrt{5}i}{10} & 0 & \frac{\sqrt{5}}{10} & 0 & 0 \\ \frac{\sqrt{5}i}{10} & 0 & \frac{\sqrt{5}}{10} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{5}}{10} & 0 & \frac{\sqrt{5}i}{5} & \frac{\sqrt{5}}{10} & 0 \\ \frac{\sqrt{5}}{10} & 0 & -\frac{\sqrt{5}i}{5} & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & -\frac{\sqrt{5}}{10} & \frac{\sqrt{5}i}{10} & 0 \end{bmatrix}$$

$$\boxed{\text{x55}}\quad \mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)=\begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} \\ 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \end{bmatrix}$$

$$\boxed{\text{x56}}\quad \mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)=\begin{bmatrix} 0 & \frac{\sqrt{3}i}{6} & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ -\frac{\sqrt{3}i}{6} & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} \\ 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \end{bmatrix}$$

$$\boxed{\text{x57}}\quad \mathbb{M}_{1}^{(1,1;a)}(A_{2g})=\begin{bmatrix} -\frac{\sqrt{30}}{30} & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{20} \\ 0 & \frac{\sqrt{30}}{30} & 0 & 0 & \frac{\sqrt{30}}{20} & 0 \\ 0 & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 & -\frac{\sqrt{30}i}{20} \\ 0 & 0 & 0 & \frac{\sqrt{30}}{30} & \frac{\sqrt{30}i}{20} & 0 \\ 0 & \frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{20} & \frac{\sqrt{30}}{15} & 0 \\ \frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{20} & 0 & 0 & -\frac{\sqrt{30}}{15} \end{bmatrix}$$

$$\boxed{\text{x58}}\quad \mathbb{M}_{1,1}^{(1,1;a)}(E_g)=\begin{bmatrix} 0 & \frac{\sqrt{30}}{15} & 0 & -\frac{\sqrt{30}i}{20} & \frac{\sqrt{30}}{20} & 0 \\ \frac{\sqrt{30}}{15} & 0 & \frac{\sqrt{30}i}{20} & 0 & 0 & -\frac{\sqrt{30}}{20} \\ 0 & -\frac{\sqrt{30}i}{20} & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 \\ \frac{\sqrt{30}i}{20} & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 & 0 \\ \frac{\sqrt{30}}{20} & 0 & 0 & 0 & 0 & -\frac{\sqrt{30}}{30} \\ 0 & -\frac{\sqrt{30}}{20} & 0 & 0 & -\frac{\sqrt{30}}{30} & 0 \end{bmatrix}$$

$\boxed{\text{x59}}$ $\mathbb{M}_{1,2}^{(1,1;a)}(E_g) = \begin{bmatrix} 0 & -\frac{\sqrt{30}i}{30} & 0 & -\frac{\sqrt{30}}{20} & 0 & 0 \\ \frac{\sqrt{30}i}{30} & 0 & -\frac{\sqrt{30}}{20} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{15} & -\frac{\sqrt{30}}{20} & 0 \\ -\frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{15} & 0 & 0 & \frac{\sqrt{30}}{20} \\ 0 & 0 & -\frac{\sqrt{30}}{20} & 0 & 0 & -\frac{\sqrt{30}i}{30} \\ 0 & 0 & 0 & \frac{\sqrt{30}}{20} & \frac{\sqrt{30}i}{30} & 0 \end{bmatrix}$

$\boxed{\text{x60}}$ $\mathbb{T}_{2}^{(1,0;a)}(A_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x61}}$ $\mathbb{T}_{2}^{(1,0;a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & \frac{\sqrt{6}}{12} & 0 \\ 0 & -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 \\ \frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x62}}$ $\mathbb{T}_{2}^{(1,0;a)}(B_{2g}) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ 0 & -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x63}}$ $\mathbb{T}_{2,1}^{(1,0;a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \end{bmatrix}$

$\boxed{\text{x64}}$ $\mathbb{T}_{2,2}^{(1,0;a)}(E_g) = \begin{bmatrix} 0 & \frac{\sqrt{6}i}{6} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$

Cluster SAMB

- Site cluster

** Wyckoff: `1a`

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

- Bond cluster

** Wyckoff: `1a@1b`

$\boxed{\text{y2}}$ $\mathbb{Q}_0^{(s)}(A_{1g}) = [1]$

$\boxed{\text{y3}}$ $\mathbb{T}_1^{(s)}(A_{2u}) = [i]$

** Wyckoff: `2b@2f`

$\boxed{\text{y4}}$ $\mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right]$

$\boxed{\text{y5}}$ $\mathbb{Q}_2^{(s)}(B_{1g}) = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}\right]$

$\boxed{\text{y6}}$ $\mathbb{T}_{1,1}^{(s)}(E_u) = [0, -i]$

$\boxed{\text{y7}}$ $\mathbb{T}_{1,2}^{(s)}(E_u) = [i, 0]$

** Wyckoff: `2c@1c`

$\boxed{\text{y8}}$ $\mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right]$

$\boxed{\text{y9}}$ $\mathbb{Q}_2^{(s)}(B_{2g}) = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}\right]$

$\boxed{\text{y10}}$ $\mathbb{T}_{1,1}^{(s)}(E_u) = \left[\frac{\sqrt{2}i}{2}, -\frac{\sqrt{2}i}{2}\right]$

$\boxed{\text{y11}}$ $\mathbb{T}_{1,2}^{(s)}(E_u) = \left[\frac{\sqrt{2}i}{2}, \frac{\sqrt{2}i}{2}\right]$

** Wyckoff: `4e@2e`

$\boxed{\text{y12}}$ $\mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$

$\boxed{\text{y13}}$ $\mathbb{T}_1^{(s)}(A_{2u}) = \left[\frac{i}{2}, \frac{i}{2}, \frac{i}{2}, \frac{i}{2}\right]$

$\boxed{\text{y14}}$ $\mathbb{Q}_2^{(s)}(B_{1g}) = \left[\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\right]$

$\boxed{\text{y15}}$ $\mathbb{M}_2^{(s)}(B_{2u}) = \left[\frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, -\frac{i}{2}\right]$

$\boxed{\text{y16}}$ $\mathbb{Q}_{2,1}^{(s)}(E_g) = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}, 0, 0\right]$

$\boxed{\text{y17}}$ $\mathbb{Q}_{2,2}^{(s)}(E_g) = \left[0, 0, -\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right]$

$\boxed{\text{y18}}$ $\mathbb{T}_{1,1}^{(s)}(E_u) = \left[0, 0, -\frac{\sqrt{2}i}{2}, \frac{\sqrt{2}i}{2}\right]$

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

Site and Bond

Table 5: Orbital of each site

#	site	orbital
1	`A`	$\lvert s,\uparrow\rangle$, $\lvert s,\downarrow\rangle$, $\lvert p_x,\uparrow\rangle$, $\lvert p_x,\downarrow\rangle$, $\lvert p_y,\uparrow\rangle$, $\lvert p_y,\downarrow\rangle$, $\lvert p_z,\uparrow\rangle$, $\lvert p_z,\downarrow\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	`A`	`A`	`[1,2,3,4]`	`[s,p]`	`[s,p]`

Site in Unit Cell

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

Table 7: '`A`' (#1) site cluster (`1a`), `4/mmm`

SL	position ($\boldsymbol{s}$)	mapping
1	`[ 0.00000, 0.00000, 0.00000]`	`[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16]`

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 8: 1-th 'A'-'A' [1] (#1) bond cluster (2b@2f), ND, $|\boldsymbol{v}|$= 1.0 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[0.00000, 1.00000, 0.00000]	[0.00000, 0.50000, 0.00000]	[1,-2,5,-6,-9,10,-13,14]	(1,1)	(1,1)	[0,-1,0]
2	[-1.00000, 0.00000, 0.00000]	[0.50000, 0.00000, 0.00000]	[3,-4,-7,8,-11,12,15,-16]	(1,1)	(1,1)	[1,0,0]

Table 9: 2-th 'A'-'A' [1] (#2) bond cluster (2c@1c), ND, $|\boldsymbol{v}|$= 1.41421 (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,-2,7,-8,-9,10,-15,16]	(1,1)	(1,1)	[1,1,0]
2	[1.00000,-1.00000, 0.00000]	[0.50000, 0.50000, 0.00000]	[3,-4,5,-6,-11,12,-13,14]	(1,1)	(1,1)	[-1,1,0]

Table 10: 3-th 'A'-'A' [1] (#3) bond cluster (1a@1b), ND, $|\boldsymbol{v}|$= 1.5 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[0.00000, 0.00000,-1.00000]	[0.00000, 0.00000, 0.50000]	[1,2,3,4,-5,-6,-7,-8,-9,-10,-11,-12,13,14,15,16]	(1,1)	(1,1)	[0,0,1]

Table 11: 4-th 'A'-'A' [1] (#4) bond cluster (4e@2e), ND, $|\boldsymbol{v}|$= 1.80278 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[0.00000, 1.00000,-1.00000]	[0.00000, 0.50000, 0.50000]	[1,-6,-9,14]	(1,1)	(1,1)	[0,-1,1]
2	[0.00000,-1.00000,-1.00000]	[0.00000, 0.50000, 0.50000]	[2,-5,-10,13]	(1,1)	(1,1)	[0,1,1]
3	[-1.00000, 0.00000,-1.00000]	[0.50000, 0.00000, 0.50000]	[3,-7,-11,15]	(1,1)	(1,1)	[1,0,1]
4	[1.00000, 0.00000,-1.00000]	[0.50000, 0.00000, 0.50000]	[4,-8,-12,16]	(1,1)	(1,1)	[-1,0,1]