

# Model for “0h1”

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

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## Group and Unit Cell

- Group: SG No. 221  $O_h^1 Pm\bar{3}m$  [cubic]
- Associated point group: PG No. 221  $O_h m\bar{3}m$  [cubic]
- Unit cell:
  - $a = 1.00000$ ,  $b = 1.00000$ ,  $c = 1.00000$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 90.0$
- Lattice vectors (conventional cell):
  - $\mathbf{a}_1 = [1.00000, 0.00000, 0.00000]$
  - $\mathbf{a}_2 = [0.00000, 1.00000, 0.00000]$
  - $\mathbf{a}_3 = [0.00000, 0.00000, 1.00000]$

Table 1: Symmetry operation

| #  | SO                   | #  | SO                   | #  | SO                  | #  | SO                   | #  | SO                   |
|----|----------------------|----|----------------------|----|---------------------|----|----------------------|----|----------------------|
| 1  | $\{1 0\}$            | 2  | $\{2_{001} 0\}$      | 3  | $\{2_{010} 0\}$     | 4  | $\{2_{100} 0\}$      | 5  | $\{3^+_{111} 0\}$    |
| 6  | $\{3^+_{-11-1} 0\}$  | 7  | $\{3^+_{1-1-1} 0\}$  | 8  | $\{3^+_{-1-11} 0\}$ | 9  | $\{3^-_{111} 0\}$    | 10 | $\{3^-_{1-1-1} 0\}$  |
| 11 | $\{3^-_{-1-11} 0\}$  | 12 | $\{3^-_{-11-1} 0\}$  | 13 | $\{2_{110} 0\}$     | 14 | $\{2_{1-10} 0\}$     | 15 | $\{4^-_{001} 0\}$    |
| 16 | $\{4^+_{001} 0\}$    | 17 | $\{4^-_{100} 0\}$    | 18 | $\{2_{011} 0\}$     | 19 | $\{2_{01-1} 0\}$     | 20 | $\{4^+_{100} 0\}$    |
| 21 | $\{4^+_{010} 0\}$    | 22 | $\{2_{101} 0\}$      | 23 | $\{4^-_{010} 0\}$   | 24 | $\{2_{-101} 0\}$     | 25 | $\{-1 0\}$           |
| 26 | $\{m_{001} 0\}$      | 27 | $\{m_{010} 0\}$      | 28 | $\{m_{100} 0\}$     | 29 | $\{-3^+_{111} 0\}$   | 30 | $\{-3^+_{-11-1} 0\}$ |
| 31 | $\{-3^+_{1-1-1} 0\}$ | 32 | $\{-3^+_{-1-11} 0\}$ | 33 | $\{-3^-_{111} 0\}$  | 34 | $\{-3^-_{1-1-1} 0\}$ | 35 | $\{-3^-_{-1-11} 0\}$ |
| 36 | $\{-3^-_{-11-1} 0\}$ | 37 | $\{m_{110} 0\}$      | 38 | $\{m_{1-10} 0\}$    | 39 | $\{-4^-_{001} 0\}$   | 40 | $\{-4^+_{001} 0\}$   |
| 41 | $\{-4^-_{100} 0\}$   | 42 | $\{m_{011} 0\}$      | 43 | $\{m_{01-1} 0\}$    | 44 | $\{-4^+_{100} 0\}$   | 45 | $\{-4^+_{010} 0\}$   |
| 46 | $\{m_{101} 0\}$      | 47 | $\{-4^-_{010} 0\}$   | 48 | $\{m_{-101} 0\}$    |    |                      |    |                      |

Table 2: Harmonics

| #  | symbol                     | irrep.   | rank | X      | multiplicity | component | symmetry   |
|----|----------------------------|----------|------|--------|--------------|-----------|--|
| 1  | $\mathbb{Q}_0(A_{1g})$     | $A_{1g}$ | 0    | $Q, T$ | -            | -         | 1  |
| 2  | $\mathbb{Q}_4(A_{1g})$     | $A_{1g}$ | 4    | $Q, T$ | -            | -         | $\frac{\sqrt{21}(x^4-3x^2y^2-3x^2z^2+y^4-3y^2z^2+z^4)}{6}$     |
| 3  | $\mathbb{G}_0(A_{1u})$     | $A_{1u}$ | 0    | $G, M$ | -            | -         | 1  |
| 4  | $\mathbb{G}_4(A_{1u})$     | $A_{1u}$ | 4    | $G, M$ | -            | -         | $\frac{\sqrt{21}(x^4-3x^2y^2-3x^2z^2+y^4-3y^2z^2+z^4)}{6}$     |
| 5  | $\mathbb{G}_3(A_{2g})$     | $A_{2g}$ | 3    | $G, M$ | -            | -         | $\sqrt{15}xyz$   |
| 6  | $\mathbb{Q}_3(A_{2u})$     | $A_{2u}$ | 3    | $Q, T$ | -            | -         | $\sqrt{15}xyz$   |
| 7  | $\mathbb{Q}_{2,1}(E_g)$    | $E_g$    | 2    | $Q, T$ | -            | 1         | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$                         |
| 8  | $\mathbb{Q}_{2,2}(E_g)$    |          |      |        |              | 2         | $\frac{\sqrt{3}(x-y)(x+y)}{2}$                                 |
| 9  | $\mathbb{Q}_{4,1}(E_g)$    | $E_g$    | 4    | $Q, T$ | -            | 1         | $-\frac{\sqrt{15}(x^4-12x^2y^2+6x^2z^2+y^4+6y^2z^2-2z^4)}{12}$ |
| 10 | $\mathbb{Q}_{4,2}(E_g)$    |          |      |        |              | 2         | $\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$                   |
| 11 | $\mathbb{G}_{2,1}(E_u)$    | $E_u$    | 2    | $G, M$ | -            | 1         | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$                         |
| 12 | $\mathbb{G}_{2,2}(E_u)$    |          |      |        |              | 2         | $\frac{\sqrt{3}(x-y)(x+y)}{2}$                                 |
| 13 | $\mathbb{G}_{4,1}(E_u)$    | $E_u$    | 4    | $G, M$ | -            | 1         | $-\frac{\sqrt{15}(x^4-12x^2y^2+6x^2z^2+y^4+6y^2z^2-2z^4)}{12}$ |
| 14 | $\mathbb{G}_{4,2}(E_u)$    |          |      |        |              | 2         | $\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$                   |
| 15 | $\mathbb{Q}_{5,1}(E_u)$    | $E_u$    | 5    | $Q, T$ | -            | 1         | $\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$                            |
| 16 | $\mathbb{Q}_{5,2}(E_u)$    |          |      |        |              | 2         | $\frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2}$                        |
| 17 | $\mathbb{G}_{1,1}(T_{1g})$ | $T_{1g}$ | 1    | $G, M$ | -            | 1         | $x$  |
| 18 | $\mathbb{G}_{1,2}(T_{1g})$ |          |      |        |              | 2         | $y$  |
| 19 | $\mathbb{G}_{1,3}(T_{1g})$ |          |      |        |              | 3         | $z$  |
| 20 | $\mathbb{G}_{3,1}(T_{1g})$ | $T_{1g}$ | 3    | $G, M$ | -            | 1         | $\frac{x(2x^2-3y^2-3z^2)}{2}$                                  |

continued ...

Table 2

| #  | symbol                        | irrep.   | rank | X      | multiplicity | component | symmetry  |
|----|-------------------------------|----------|------|--------|--------------|-----------|---|
| 21 | $\mathbb{G}_{3,2}(T_{1g})$    |          |      |        |              | 2         | $-\frac{y(3x^2-2y^2+3z^2)}{2}$                    |
| 22 | $\mathbb{G}_{3,3}(T_{1g})$    |          |      |        |              | 3         | $-\frac{z(3x^2+3y^2-2z^2)}{2}$                    |
| 23 | $\mathbb{Q}_{4,1}(T_{1g})$    | $T_{1g}$ | 4    | $Q, T$ | -            | 1         | $\frac{\sqrt{35}yz(y-z)(y+z)}{2}$                 |
| 24 | $\mathbb{Q}_{4,2}(T_{1g})$    |          |      |        |              | 2         | $-\frac{\sqrt{35}xz(x-z)(x+z)}{2}$                |
| 25 | $\mathbb{Q}_{4,3}(T_{1g})$    |          |      |        |              | 3         | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$                 |
| 26 | $\mathbb{Q}_{1,1}(T_{1u})$    | $T_{1u}$ | 1    | $Q, T$ | -            | 1         | $x$   |
| 27 | $\mathbb{Q}_{1,2}(T_{1u})$    |          |      |        |              | 2         | $y$   |
| 28 | $\mathbb{Q}_{1,3}(T_{1u})$    |          |      |        |              | 3         | $z$   |
| 29 | $\mathbb{Q}_{3,1}(T_{1u})$    | $T_{1u}$ | 3    | $Q, T$ | -            | 1         | $\frac{x(2x^2-3y^2-3z^2)}{2}$                     |
| 30 | $\mathbb{Q}_{3,2}(T_{1u})$    |          |      |        |              | 2         | $-\frac{y(3x^2-2y^2+3z^2)}{2}$                    |
| 31 | $\mathbb{Q}_{3,3}(T_{1u})$    |          |      |        |              | 3         | $-\frac{z(3x^2+3y^2-2z^2)}{2}$                    |
| 32 | $\mathbb{G}_{4,1}(T_{1u})$    | $T_{1u}$ | 4    | $G, M$ | -            | 1         | $\frac{\sqrt{35}yz(y-z)(y+z)}{2}$                 |
| 33 | $\mathbb{G}_{4,2}(T_{1u})$    |          |      |        |              | 2         | $-\frac{\sqrt{35}xz(x-z)(x+z)}{2}$                |
| 34 | $\mathbb{G}_{4,3}(T_{1u})$    |          |      |        |              | 3         | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$                 |
| 35 | $\mathbb{Q}_{5,1}(T_{1u}, 2)$ | $T_{1u}$ | 5    | $Q, T$ | 2            | 1         | $\frac{3\sqrt{35}x(y^2-2yz-z^2)(y^2+2yz-z^2)}{8}$ |
| 36 | $\mathbb{Q}_{5,2}(T_{1u}, 2)$ |          |      |        |              | 2         | $\frac{3\sqrt{35}y(x^2-2xz-z^2)(x^2+2xz-z^2)}{8}$ |
| 37 | $\mathbb{Q}_{5,3}(T_{1u}, 2)$ |          |      |        |              | 3         | $\frac{3\sqrt{35}z(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$ |
| 38 | $\mathbb{Q}_{2,1}(T_{2g})$    | $T_{2g}$ | 2    | $Q, T$ | -            | 1         | $\sqrt{3}yz$                                      |
| 39 | $\mathbb{Q}_{2,2}(T_{2g})$    |          |      |        |              | 2         | $\sqrt{3}xz$                                      |
| 40 | $\mathbb{Q}_{2,3}(T_{2g})$    |          |      |        |              | 3         | $\sqrt{3}xy$                                      |
| 41 | $\mathbb{G}_{3,1}(T_{2g})$    | $T_{2g}$ | 3    | $G, M$ | -            | 1         | $\frac{\sqrt{15}x(y-z)(y+z)}{2}$                  |

continued ...

Table 2

| #  | symbol                     | irrep.   | rank | X      | multiplicity | component | symmetry   |
|----|----------------------------|----------|------|--------|--------------|-----------|--|
| 42 | $\mathbb{G}_{3,2}(T_{2g})$ |          |      |        |              | 2         | $-\frac{\sqrt{15}y(x-z)(x+z)}{2}$                |
| 43 | $\mathbb{G}_{3,3}(T_{2g})$ |          |      |        |              | 3         | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$                 |
| 44 | $\mathbb{Q}_{4,1}(T_{2g})$ | $T_{2g}$ | 4    | $Q, T$ | -            | 1         | $\frac{\sqrt{5}yz(6x^2-y^2-z^2)}{2}$             |
| 45 | $\mathbb{Q}_{4,2}(T_{2g})$ |          |      |        |              | 2         | $-\frac{\sqrt{5}xz(x^2-6y^2+z^2)}{2}$            |
| 46 | $\mathbb{Q}_{4,3}(T_{2g})$ |          |      |        |              | 3         | $-\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$            |
| 47 | $\mathbb{G}_{2,1}(T_{2u})$ | $T_{2u}$ | 2    | $G, M$ | -            | 1         | $\sqrt{3}yz$                                     |
| 48 | $\mathbb{G}_{2,2}(T_{2u})$ |          |      |        |              | 2         | $\sqrt{3}xz$                                     |
| 49 | $\mathbb{G}_{2,3}(T_{2u})$ |          |      |        |              | 3         | $\sqrt{3}xy$                                     |
| 50 | $\mathbb{Q}_{3,1}(T_{2u})$ | $T_{2u}$ | 3    | $Q, T$ | -            | 1         | $\frac{\sqrt{15}x(y-z)(y+z)}{2}$                 |
| 51 | $\mathbb{Q}_{3,2}(T_{2u})$ |          |      |        |              | 2         | $-\frac{\sqrt{15}y(x-z)(x+z)}{2}$                |
| 52 | $\mathbb{Q}_{3,3}(T_{2u})$ |          |      |        |              | 3         | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$                 |
| 53 | $\mathbb{G}_{4,1}(T_{2u})$ | $T_{2u}$ | 4    | $G, M$ | -            | 1         | $\frac{\sqrt{5}yz(6x^2-y^2-z^2)}{2}$             |
| 54 | $\mathbb{G}_{4,2}(T_{2u})$ |          |      |        |              | 2         | $-\frac{\sqrt{5}xz(x^2-6y^2+z^2)}{2}$            |
| 55 | $\mathbb{G}_{4,3}(T_{2u})$ |          |      |        |              | 3         | $-\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$            |
| 56 | $\mathbb{Q}_{5,1}(T_{2u})$ | $T_{2u}$ | 5    | $Q, T$ | -            | 1         | $\frac{\sqrt{105}x(y-z)(y+z)(2x^2-y^2-z^2)}{4}$  |
| 57 | $\mathbb{Q}_{5,2}(T_{2u})$ |          |      |        |              | 2         | $\frac{\sqrt{105}y(x-z)(x+z)(x^2-2y^2+z^2)}{4}$  |
| 58 | $\mathbb{Q}_{5,3}(T_{2u})$ |          |      |        |              | 3         | $-\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$ |

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Basis in full matrix

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Table 3: dimension = 8

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

Table 4: Atomic basis (orbital part only)

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

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**SAMB**


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604 (all 604) SAMBs

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

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**

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

$$\boxed{\text{z300}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z301}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z362}} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z363}} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}) = \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z364}} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}) = \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z365}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(T_{1u}) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z366}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(T_{1u}) = \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z367}} \quad \mathbb{Q}_{1,3}^{(1,0;c)}(T_{1u}) = \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z485}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z486}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{3}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z487}} \quad \mathbb{G}_{2,3}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{3}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

- '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**

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

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

$$\boxed{\text{z30}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z31}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z32}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z33}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z86}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(T_{1g}) = \frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z87}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(T_{1g}) = \frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z88}} \quad \mathbb{G}_{1,3}^{(1,0;c)}(T_{1g}) = \frac{\sqrt{3}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z170}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z171}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z172}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z173}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$



$$\boxed{\text{z174}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z175}} \quad \mathbb{Q}_{2,3}^{(1,-1;c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

• 'A'-'A' bond-cluster : **A;A\_001\_1**

\* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$

\* ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$

\* wyckoff: **3a@3d**

$$\boxed{\text{z4}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z34}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z35}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z270}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z302}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z303}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2}$$

$$\boxed{\text{z368}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}) = \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z369}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z370}} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z488}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z489}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z490}} \quad \mathbb{G}_{2,3}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

• '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: **3a@3d**

$$\boxed{\text{z5}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) = \frac{\sqrt{3}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z6}} \quad \mathbb{Q}_0^{(1,0;c)}(A_{1g}) = \frac{\sqrt{3}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z21}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z36}} \quad \mathbb{G}_0^{(1,1;c)}(A_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z37}} \quad \mathbb{G}_3^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z38}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z39}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = -\frac{\sqrt{3}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z40}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2}$$

$$\boxed{\text{z41}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = -\frac{\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} + \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2}$$

$$\boxed{\text{z89}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = -\frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z90}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g) = -\frac{\sqrt{3}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z91}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g) = \frac{\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2}$$

$$\boxed{\text{z92}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, a) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z93}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, a) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z94}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, b) = \frac{\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z95}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, b) = -\frac{\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z96}} \quad \mathbb{G}_{2,1}^{(1,1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z97}} \quad \mathbb{G}_{2,2}^{(1,1;c)}(E_u) = \frac{\sqrt{2}\mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z98}} \quad \mathbb{G}_{1,1}^{(c)}(T_{1g}) = \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z99}} \quad \mathbb{G}_{1,2}^{(c)}(T_{1g}) = -\frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z100}} \quad \mathbb{G}_{1,3}^{(c)}(T_{1g}) = \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z101}} \quad \mathbb{G}_{1,1}^{(1,-1;c)}(T_{1g}) = -\frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{30} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10}$$

$$\boxed{\text{z102}} \quad \mathbb{G}_{1,2}^{(1,-1;c)}(T_{1g}) = -\frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{30} + \frac{\sqrt{10}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{10} - \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10}$$

$$\boxed{\text{z103}} \quad \mathbb{G}_{1,3}^{(1,-1;c)}(T_{1g}) = \frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} + \frac{\sqrt{10}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10}$$

$$\begin{aligned}
\text{z176} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(T_{1g}) &= -\frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} + \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{15} \\
\text{z177} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(T_{1g}) &= -\frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{15} \\
\text{z178} \quad \mathbb{G}_{3,3}^{(1,-1;c)}(T_{1g}) &= \frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{5} - \frac{\sqrt{15}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{15} \\
\text{z179} \quad \mathbb{G}_{1,1}^{(1,0;c)}(T_{1g}) &= \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\text{z180} \quad \mathbb{G}_{1,2}^{(1,0;c)}(T_{1g}) &= -\frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z181} \quad \mathbb{G}_{1,3}^{(1,0;c)}(T_{1g}) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z182} \quad \mathbb{G}_{1,1}^{(1,1;c)}(T_{1g}) &= \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\text{z183} \quad \mathbb{G}_{1,2}^{(1,1;c)}(T_{1g}) &= \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} \\
\text{z184} \quad \mathbb{G}_{1,3}^{(1,1;c)}(T_{1g}) &= \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z185} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z186} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z187} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z271} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}, b) &= -\frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z272} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}, b) &= -\frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z287}} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}, b) &= \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} \\
\boxed{\text{z304}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}) &= \frac{\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{3}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\boxed{\text{z305}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}) &= -\frac{\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{3}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\boxed{\text{z306}} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}) &= -\frac{\sqrt{3}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\boxed{\text{z307}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z308}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z309}} \quad \mathbb{Q}_{1,3}^{(1,0;c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z371}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(T_{1u}, b) &= -\frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\boxed{\text{z372}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(T_{1u}, b) &= -\frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\boxed{\text{z373}} \quad \mathbb{Q}_{1,3}^{(1,0;c)}(T_{1u}, b) &= \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} \\
\boxed{\text{z374}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z375}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z376}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z377}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{2}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}
\end{aligned}$$

$$\begin{aligned}
\text{z378} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(T_{2g}) &= -\frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{2}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z379} \quad \mathbb{Q}_{2,3}^{(1,-1;c)}(T_{2g}) &= -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z380} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\text{z381} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z382} \quad \mathbb{Q}_{2,3}^{(1,0;c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z383} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(T_{2g}) &= -\frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} \\
\text{z384} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} - \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\text{z385} \quad \mathbb{G}_{3,3}^{(1,-1;c)}(T_{2g}) &= -\frac{\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\text{z491} \quad \mathbb{Q}_{3,1}^{(c)}(T_{2u}) &= -\frac{\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\text{z492} \quad \mathbb{Q}_{3,2}^{(c)}(T_{2u}) &= \frac{\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\text{z493} \quad \mathbb{Q}_{3,3}^{(c)}(T_{2u}) &= \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\text{z494} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{2u}) &= -\frac{\sqrt{3}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z495} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{2u}) &= -\frac{\sqrt{3}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z496} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{3}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{3}
\end{aligned}$$

$$\boxed{\text{z497}} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{2u}) = -\frac{\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z498}} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{2u}) = \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z499}} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{2u}) = \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3}$$

$$\boxed{\text{z500}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z501}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{3}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z502}} \quad \mathbb{G}_{2,3}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{3}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

• '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: **3aQ3d**

$$\boxed{\text{z7}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z8}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

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

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

$$\boxed{\text{z22}} \quad \mathbb{G}_0^{(c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z23}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z42}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z43}} \quad \mathbb{G}_0^{(1,1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z44}} \quad \mathbb{G}_3^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z45}} \quad \mathbb{G}_3^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z46}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} - \frac{\sqrt{3}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z47}} \quad \mathbb{Q}_3^{(1,0;c)}(A_{2u}) = \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z48}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z49}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z50}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z51}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z52}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, c) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z53}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, c) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z104}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z105}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$



$$\begin{aligned}
\text{z106} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, b) &= \frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z107} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, b) &= -\frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} \\
\text{z108} \quad \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} \\
\text{z109} \quad \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} \\
\text{z110} \quad \mathbb{G}_{2,1}^{(c)}(E_u) &= -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z111} \quad \mathbb{G}_{2,2}^{(c)}(E_u) &= \frac{\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z112} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, a) &= -\frac{\sqrt{42}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{70}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{42}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} + \frac{\sqrt{70}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{14} \\
\text{z113} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, a) &= \frac{3\sqrt{14}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{210}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{84} - \frac{3\sqrt{14}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} - \frac{\sqrt{210}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{84} + \frac{\sqrt{210}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{42} \\
\text{z114} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, b) &= -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z115} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, b) &= \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z188} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(E_u) &= -\frac{\sqrt{210}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{84} + \frac{3\sqrt{14}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{210}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{84} - \frac{3\sqrt{14}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} + \frac{\sqrt{210}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{42} \\
\text{z189} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(E_u) &= \frac{\sqrt{70}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{70}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} - \frac{\sqrt{42}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{14} \\
\text{z190} \quad \mathbb{G}_{2,1}^{(1,0;c)}(E_u) &= -\frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z191} \quad \mathbb{G}_{2,2}^{(1,0;c)}(E_u) &= -\frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}
\end{aligned}$$

$$\boxed{\text{z192}} \quad \mathbb{G}_{2,1}^{(1,1;c)}(E_u) = -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z193}} \quad \mathbb{G}_{2,2}^{(1,1;c)}(E_u) = \frac{\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2}$$

$$\boxed{\text{z194}} \quad \mathbb{Q}_{4,1}^{(c)}(T_{1g}) = -\frac{\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z195}} \quad \mathbb{Q}_{4,2}^{(c)}(T_{1g}) = \frac{\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z196}} \quad \mathbb{Q}_{4,3}^{(c)}(T_{1g}) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3}$$

$$\boxed{\text{z197}} \quad \mathbb{Q}_{4,1}^{(1,-1;c)}(T_{1g}) = -\frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z198}} \quad \mathbb{Q}_{4,2}^{(1,-1;c)}(T_{1g}) = \frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z199}} \quad \mathbb{Q}_{4,3}^{(1,-1;c)}(T_{1g}) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3}$$

$$\boxed{\text{z200}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(T_{1g}, a) = \frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z201}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(T_{1g}, a) = \frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z202}} \quad \mathbb{G}_{1,3}^{(1,0;c)}(T_{1g}, a) = \frac{\sqrt{3}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z273}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(T_{1g}, b) = -\frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z274}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(T_{1g}, b) = -\frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z275}} \quad \mathbb{G}_{1,3}^{(1,0;c)}(T_{1g}, b) = \frac{\sqrt{3}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{3}$$

$$\begin{aligned}
\text{z276} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\text{z288} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z289} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z310} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\text{z311} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z312} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z313} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{1u}) &= -\frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} \\
\text{z314} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{1u}) &= \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} \\
\text{z315} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{1u}) &= -\frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} \\
\text{z316} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(T_{1u}) &= -\frac{\sqrt{30}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{30} + \frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} \\
\text{z317} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(T_{1u}) &= -\frac{\sqrt{30}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{30} + \frac{\sqrt{10}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{10} - \frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} \\
\text{z318} \quad \mathbb{Q}_{1,3}^{(1,0;c)}(T_{1u}) &= \frac{\sqrt{30}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} + \frac{\sqrt{10}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} \\
\text{z319} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{1u}) &= -\frac{\sqrt{5}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} + \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{15} \\
\text{z320} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{1u}) &= -\frac{\sqrt{5}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{15}
\end{aligned}$$

$$\begin{aligned}
\text{z321} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{1u}) &= \frac{\sqrt{5}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{5} - \frac{\sqrt{15}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{15} \\
\text{z386} \quad \mathbb{Q}_{1,1}^{(1,1;c)}(T_{1u}) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\text{z387} \quad \mathbb{Q}_{1,2}^{(1,1;c)}(T_{1u}) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z388} \quad \mathbb{Q}_{1,3}^{(1,1;c)}(T_{1u}) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z389} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(T_{1u}) &= \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{4} \\
\text{z390} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(T_{1u}) &= -\frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{4} + \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{4} \\
\text{z391} \quad \mathbb{G}_{4,3}^{(1,-1;c)}(T_{1u}) &= \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{4} \\
\text{z392} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z393} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z394} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z395} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, b) &= \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z396} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, b) &= \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z397} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, b) &= -\frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} \\
\text{z398} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z399}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z400}} \quad \mathbb{Q}_{2,3}^{(1,-1;c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z401}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(T_{2g}, b) &= \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\boxed{\text{z402}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(T_{2g}, b) &= \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\boxed{\text{z403}} \quad \mathbb{Q}_{2,3}^{(1,-1;c)}(T_{2g}, b) &= -\frac{\sqrt{3}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} \\
\boxed{\text{z404}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(T_{2g}) &= -\frac{\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\boxed{\text{z405}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(T_{2g}) &= \frac{\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\boxed{\text{z406}} \quad \mathbb{Q}_{2,3}^{(1,0;c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\boxed{\text{z503}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\boxed{\text{z504}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} \\
\boxed{\text{z505}} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\boxed{\text{z506}} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{2u}) &= -\frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} \\
\boxed{\text{z507}} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{2u}) &= \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\boxed{\text{z508}} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{2u}) &= -\frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3}
\end{aligned}$$



$$\boxed{\text{z523}} \quad \mathbb{G}_{2,3}^{(1,0;c)}(T_{2u}) = -\frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z524}} \quad \mathbb{G}_{2,1}^{(1,1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z525}} \quad \mathbb{G}_{2,2}^{(1,1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z526}} \quad \mathbb{G}_{2,3}^{(1,1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

• 'A'-'A' bond-cluster : **A;A\_002\_1**

\* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$

\* ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$

\* wyckoff: **6b03c**

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

$$\boxed{\text{z54}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z55}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z203}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z204}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z205}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, a) = -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z277}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, a) = \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2}$$

$$\boxed{\text{z290}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, b) = \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2}$$

$$\begin{aligned}
\text{z322} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, b) &= \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\text{z323} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}, a) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\text{z324} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}, a) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z325} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}, a) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z407} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\text{z408} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z409} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z410} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} \\
\text{z411} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} \\
\text{z412} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} \\
\text{z527} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\text{z528} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{2u}) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z529} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z530} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}
\end{aligned}$$



$$\boxed{\text{z531}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z532}} \quad \mathbb{G}_{2,3}^{(1,-1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

• '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: **6b@3c**

$$\boxed{\text{z12}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) = \frac{\sqrt{3}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z13}} \quad \mathbb{Q}_0^{(1,-1;c)}(A_{1g}) = \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z14}} \quad \mathbb{Q}_0^{(1,0;c)}(A_{1g}) = \frac{\sqrt{3}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z24}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{5}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{5} + \frac{\sqrt{5}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{5} + \frac{\sqrt{5}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{5}$$

$$\boxed{\text{z25}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{30}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{30}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{30}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15}$$

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

$$\boxed{\text{z56}} \quad \mathbb{G}_3^{(c)}(A_{2g}) = \frac{\sqrt{3}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z57}} \quad \mathbb{G}_3^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z58}} \quad \mathbb{G}_3^{(1,0;c)}(A_{2g}) = \frac{\sqrt{3}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z59}} \quad \mathbb{Q}_3^{(c)}(A_{2u}) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3}$$

$$\begin{aligned}
\text{z60} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u}) &= \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} \\
\text{z61} \quad \mathbb{Q}_3^{(1,0;c)}(A_{2u}) &= \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} \\
\text{z62} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, a) &= -\frac{\sqrt{3}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z63} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) &= \frac{\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z64} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) &= \frac{\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} - \frac{\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2} \\
\text{z65} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) &= \frac{\sqrt{3}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{3}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\text{z66} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, a) &= -\frac{\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} + \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z67} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, a) &= -\frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z116} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, b) &= \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{3}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\text{z117} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, b) &= -\frac{\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} + \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2} \\
\text{z118} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g, a) &= -\frac{\sqrt{3}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z119} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g, a) &= \frac{\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z120} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g, b) &= \frac{\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} - \frac{\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2} \\
\text{z121} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g, b) &= \frac{\sqrt{3}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\sqrt{3}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{3}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}
\end{aligned}$$

$$\begin{aligned}
\text{z122} \quad \mathbb{G}_{2,1}^{(c)}(E_u) &= \frac{\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{2} - \frac{\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{2} \\
\text{z123} \quad \mathbb{G}_{2,2}^{(c)}(E_u) &= \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} - \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} \\
\text{z124} \quad \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} \\
\text{z125} \quad \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} \\
\text{z126} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, b) &= \frac{\sqrt{7}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{7}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} + \frac{\sqrt{7}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{7} \\
\text{z127} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, b) &= -\frac{\sqrt{7}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} - \frac{\sqrt{21}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{21}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} \\
\text{z128} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(E_u) &= \frac{\sqrt{21}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} - \frac{\sqrt{21}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} + \frac{2\sqrt{21}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} \\
\text{z129} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(E_u) &= -\frac{\sqrt{21}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{7}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{7} - \frac{\sqrt{21}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{7}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{7} \\
\text{z130} \quad \mathbb{G}_{2,1}^{(1,0;c)}(E_u) &= \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{2} - \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{2} \\
\text{z131} \quad \mathbb{G}_{2,2}^{(1,0;c)}(E_u) &= \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} - \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} \\
\text{z132} \quad \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} \\
\text{z133} \quad \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} \\
\text{z134} \quad \mathbb{Q}_{4,1}^{(1,-1;c)}(T_{1g}) &= -\frac{\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} - \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z135} \quad \mathbb{Q}_{4,2}^{(1,-1;c)}(T_{1g}) &= \frac{\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2} - \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6}
\end{aligned}$$

$$\boxed{\text{z136}} \quad \mathbb{Q}_{4,3}^{(1,-1;c)}(T_{1g}) = \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z137}} \quad \mathbb{G}_{1,1}^{(c)}(T_{1g}, a) = \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z138}} \quad \mathbb{G}_{1,2}^{(c)}(T_{1g}, a) = -\frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z139}} \quad \mathbb{G}_{1,3}^{(c)}(T_{1g}, a) = \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z140}} \quad \mathbb{G}_{1,1}^{(c)}(T_{1g}, b) = \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z141}} \quad \mathbb{G}_{1,2}^{(c)}(T_{1g}, b) = \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z142}} \quad \mathbb{G}_{1,3}^{(c)}(T_{1g}, b) = \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z206}} \quad \mathbb{G}_{1,1}^{(1,-1;c)}(T_{1g}, a) = -\frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{30} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10}$$

$$\boxed{\text{z207}} \quad \mathbb{G}_{1,2}^{(1,-1;c)}(T_{1g}, a) = -\frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{30} + \frac{\sqrt{10}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{10} - \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10}$$

$$\boxed{\text{z208}} \quad \mathbb{G}_{1,3}^{(1,-1;c)}(T_{1g}, a) = \frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} + \frac{\sqrt{10}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10}$$

$$\boxed{\text{z209}} \quad \mathbb{G}_{1,1}^{(1,-1;c)}(T_{1g}, b) = -\frac{\sqrt{6}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z210}} \quad \mathbb{G}_{1,2}^{(1,-1;c)}(T_{1g}, b) = \frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z211}} \quad \mathbb{G}_{1,3}^{(1,-1;c)}(T_{1g}, b) = -\frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z212}} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(T_{1g}) = -\frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} + \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{15}$$

$$\begin{aligned}
\text{z213} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(T_{1g}) &= -\frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{15} \\
\text{z214} \quad \mathbb{G}_{3,3}^{(1,-1;c)}(T_{1g}) &= \frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{5} - \frac{\sqrt{15}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{15} \\
\text{z215} \quad \mathbb{G}_{1,1}^{(1,0;c)}(T_{1g}, a) &= \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\text{z216} \quad \mathbb{G}_{1,2}^{(1,0;c)}(T_{1g}, a) &= -\frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z217} \quad \mathbb{G}_{1,3}^{(1,0;c)}(T_{1g}, a) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z218} \quad \mathbb{G}_{1,1}^{(1,0;c)}(T_{1g}, b) &= \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\text{z219} \quad \mathbb{G}_{1,2}^{(1,0;c)}(T_{1g}, b) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z220} \quad \mathbb{G}_{1,3}^{(1,0;c)}(T_{1g}, b) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z221} \quad \mathbb{G}_{1,1}^{(1,1;c)}(T_{1g}) &= \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\text{z222} \quad \mathbb{G}_{1,2}^{(1,1;c)}(T_{1g}) &= \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} \\
\text{z223} \quad \mathbb{G}_{1,3}^{(1,1;c)}(T_{1g}) &= \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z224} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z225} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z226} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3}
\end{aligned}$$

$$\boxed{\text{z227}} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}, b) = -\frac{\sqrt{30}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} + \frac{\sqrt{10}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{10}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10}$$

$$\boxed{\text{z228}} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}, b) = \frac{\sqrt{10}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{10} - \frac{\sqrt{30}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} - \frac{\sqrt{10}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{10}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10}$$

$$\boxed{\text{z229}} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}, b) = \frac{\sqrt{10}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} + \frac{\sqrt{30}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{15}$$

$$\boxed{\text{z230}} \quad \mathbb{Q}_{3,1}^{(c)}(T_{1u}) = -\frac{\sqrt{5}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} - \frac{\sqrt{15}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15}$$

$$\boxed{\text{z231}} \quad \mathbb{Q}_{3,2}^{(c)}(T_{1u}) = -\frac{\sqrt{15}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} - \frac{\sqrt{5}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15}$$

$$\boxed{\text{z232}} \quad \mathbb{Q}_{3,3}^{(c)}(T_{1u}) = -\frac{\sqrt{15}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{15}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{5}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5}$$

$$\boxed{\text{z278}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}) = -\frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} \\ - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30}$$

$$\boxed{\text{z279}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}) = \frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} + \frac{\sqrt{30}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} \\ - \frac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{30}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30}$$

$$\boxed{\text{z280}} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}) = -\frac{\sqrt{30}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{15}$$

$$\boxed{\text{z291}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{1u}) = \frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{20} - \frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} - \frac{\sqrt{30}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{60} \\ + \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{60} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15}$$

$$\boxed{\text{z292}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{1u}) = -\frac{\sqrt{10}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{20} + \frac{\sqrt{30}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{60} \\ + \frac{\sqrt{10}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{60} - \frac{\sqrt{30}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15}$$

$$\begin{aligned}
\boxed{\text{z293}} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{1u}) &= -\frac{\sqrt{30}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} \\
\boxed{\text{z326}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z327}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z328}} \quad \mathbb{Q}_{1,3}^{(1,0;c)}(T_{1u}, a) &= \frac{\sqrt{3}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z329}} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(T_{1u}, b) &= -\frac{\sqrt{30}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} + \frac{\sqrt{10}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{10}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} \\
\boxed{\text{z330}} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(T_{1u}, b) &= \frac{\sqrt{10}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{10} - \frac{\sqrt{30}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} - \frac{\sqrt{10}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{10}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} \\
\boxed{\text{z331}} \quad \mathbb{Q}_{1,3}^{(1,0;c)}(T_{1u}, b) &= \frac{\sqrt{10}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} + \frac{\sqrt{30}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{15} \\
\boxed{\text{z332}} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{1u}) &= -\frac{\sqrt{5}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} - \frac{\sqrt{15}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z333}} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{1u}) &= -\frac{\sqrt{15}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} - \frac{\sqrt{5}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z334}} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{1u}) &= -\frac{\sqrt{15}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{15}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{5}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} \\
\boxed{\text{z335}} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(T_{1u}) &= -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{4} - \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{12} \\
\boxed{\text{z336}} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(T_{1u}) &= \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{4} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{12} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} \\
\boxed{\text{z337}} \quad \mathbb{G}_{4,3}^{(1,-1;c)}(T_{1u}) &= \frac{\sqrt{6}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\boxed{\text{z413}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, a) &= \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}
\end{aligned}$$

$$\boxed{\text{z414}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, a) = \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z415}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, a) = \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z416}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, b) = -\frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z417}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, b) = \frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,3}^{(a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z418}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, b) = -\frac{\sqrt{6}\mathbb{T}_{1,1}^{(a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,2}^{(a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z419}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(T_{2g}, a) = \frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{2}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z420}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(T_{2g}, a) = -\frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{2}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z421}} \quad \mathbb{Q}_{2,3}^{(1,-1;c)}(T_{2g}, a) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z422}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(T_{2g}, b) = \frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{30} - \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{10}$$

$$\boxed{\text{z423}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(T_{2g}, b) = \frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{30} + \frac{\sqrt{10}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{10}$$

$$\boxed{\text{z424}} \quad \mathbb{Q}_{2,3}^{(1,-1;c)}(T_{2g}, b) = -\frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_{2,3}^{(b)}(T_{2u})}{15} + \frac{\sqrt{10}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{10} + \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{10}$$

$$\boxed{\text{z425}} \quad \mathbb{Q}_{4,1}^{(1,-1;c)}(T_{2g}) = -\frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{10} + \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{10} + \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{15} + \frac{\sqrt{15}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{15}$$

$$\boxed{\text{z426}} \quad \mathbb{Q}_{4,2}^{(1,-1;c)}(T_{2g}) = -\frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{10} + \frac{\sqrt{15}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{15} - \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{10} + \frac{\sqrt{15}\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{15}$$

$$\boxed{\text{z427}} \quad \mathbb{Q}_{4,3}^{(1,-1;c)}(T_{2g}) = \frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_{2,3}^{(b)}(T_{2u})}{5} + \frac{\sqrt{15}\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{15} + \frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{15}$$



$$\begin{aligned}
\text{z428} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(T_{2g}, a) &= \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\text{z429} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(T_{2g}, a) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z430} \quad \mathbb{Q}_{2,3}^{(1,0;c)}(T_{2g}, a) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z431} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(T_{2g}, b) &= -\frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\text{z432} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(T_{2g}, b) &= \frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{T}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z433} \quad \mathbb{Q}_{2,3}^{(1,0;c)}(T_{2g}, b) &= -\frac{\sqrt{6}\mathbb{T}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z434} \quad \mathbb{Q}_{2,1}^{(1,1;c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} \\
\text{z435} \quad \mathbb{Q}_{2,2}^{(1,1;c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} \\
\text{z436} \quad \mathbb{Q}_{2,3}^{(1,1;c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{M}_0^{(1,1;a)}(A_{1u})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\text{z437} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(T_{2g}) &= -\frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} \\
\text{z438} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} - \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\text{z439} \quad \mathbb{G}_{3,3}^{(1,-1;c)}(T_{2g}) &= -\frac{\mathbb{M}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\mathbb{M}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\text{z533} \quad \mathbb{Q}_{3,1}^{(c)}(T_{2u}) &= -\frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} - \frac{\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} \\
\text{z534} \quad \mathbb{Q}_{3,2}^{(c)}(T_{2u}) &= -\frac{\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3}
\end{aligned}$$

$$\begin{aligned}
\text{z535} \quad \mathbb{Q}_{3,3}^{(c)}(T_{2u}) &= \frac{\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} - \frac{\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} + \frac{\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\text{z536} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{12} - \frac{\sqrt{6}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{2}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{4} \\
\text{z537} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{12} + \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{4} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} \\
\text{z538} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{2u}) &= -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} \\
\text{z539} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{2u}) &= -\frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} - \frac{\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} \\
\text{z540} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{2u}) &= -\frac{\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} \\
\text{z541} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{2u}) &= \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} - \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} + \frac{\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\text{z542} \quad \mathbb{G}_{2,1}^{(c)}(T_{2u}) &= -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} \\
\text{z543} \quad \mathbb{G}_{2,2}^{(c)}(T_{2u}) &= \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} \\
\text{z544} \quad \mathbb{G}_{2,3}^{(c)}(T_{2u}) &= -\frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_{1,3}^{(a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\text{z545} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(T_{2u}, a) &= \frac{\sqrt{3}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z546} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(T_{2u}, a) &= \frac{\sqrt{3}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z547} \quad \mathbb{G}_{2,3}^{(1,-1;c)}(T_{2u}, a) &= \frac{\sqrt{3}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_0^{(b)}(A_{1g})}{3}
\end{aligned}$$

$$\begin{aligned}
\text{z548} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(T_{2u}, b) &= \frac{\sqrt{42}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{42} + \frac{\sqrt{42}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} - \frac{\sqrt{14}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} \\
&\quad - \frac{\sqrt{14}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} \\
\text{z549} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(T_{2u}, b) &= \frac{\sqrt{42}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{42} + \frac{\sqrt{14}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} \\
&\quad + \frac{\sqrt{42}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} + \frac{\sqrt{14}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{14}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} \\
\text{z550} \quad \mathbb{G}_{2,3}^{(1,-1;c)}(T_{2u}, b) &= -\frac{\sqrt{42}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} + \frac{\sqrt{14}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{42}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} \\
\text{z551} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(T_{2u}) &= -\frac{\sqrt{14}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{28} - \frac{\sqrt{14}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} + \frac{\sqrt{42}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} \\
&\quad + \frac{\sqrt{42}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{28} + \frac{\sqrt{42}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} + \frac{\sqrt{42}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} \\
\text{z552} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(T_{2u}) &= -\frac{\sqrt{14}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{28} + \frac{\sqrt{42}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} - \frac{\sqrt{42}\mathbb{G}_{2,2}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{28} \\
&\quad - \frac{\sqrt{14}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{42}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{\sqrt{42}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} \\
\text{z553} \quad \mathbb{G}_{4,3}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{14}\mathbb{G}_{2,1}^{(1,-1;a)}(E_u)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{42}\mathbb{G}_{2,1}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} + \frac{\sqrt{42}\mathbb{G}_{2,2}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} + \frac{\sqrt{14}\mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} \\
\text{z554} \quad \mathbb{G}_{2,1}^{(1,0;c)}(T_{2u}) &= -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} \\
\text{z555} \quad \mathbb{G}_{2,2}^{(1,0;c)}(T_{2u}) &= \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} \\
\text{z556} \quad \mathbb{G}_{2,3}^{(1,0;c)}(T_{2u}) &= -\frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\text{z557} \quad \mathbb{G}_{2,1}^{(1,1;c)}(T_{2u}) &= \frac{\sqrt{3}\mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} \\
\text{z558} \quad \mathbb{G}_{2,2}^{(1,1;c)}(T_{2u}) &= \frac{\sqrt{3}\mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3}
\end{aligned}$$

$$\boxed{\text{z559}} \quad \mathbb{G}_{2,3}^{(1,1;c)}(T_{2u}) = \frac{\sqrt{3}\mathbb{G}_0^{(1,1;a)}(A_{1u})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3}$$

• '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: **6b03c**

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

$$\boxed{\text{z16}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{5}$$

$$\boxed{\text{z17}} \quad \mathbb{Q}_4^{(c)}(A_{1g}) = \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15}$$

$$\boxed{\text{z18}} \quad \mathbb{Q}_0^{(1,-1;c)}(A_{1g}) = \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{5}$$

$$\boxed{\text{z19}} \quad \mathbb{Q}_4^{(1,-1;c)}(A_{1g}) = \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15}$$

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

$$\boxed{\text{z27}} \quad \mathbb{G}_0^{(c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z28}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z29}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{1u}, a) = \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z68}} \quad \mathbb{G}_4^{(1,-1;c)}(A_{1u}, b) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} - \frac{\sqrt{3}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z69}} \quad \mathbb{G}_0^{(1,0;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z70}} \quad \mathbb{G}_0^{(1,1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z71}} \quad \mathbb{G}_3^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z72}} \quad \mathbb{G}_3^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z73}} \quad \mathbb{G}_3^{(1,0;c)}(A_{2g}) = \frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3}$$

$$\boxed{\text{z74}} \quad \mathbb{Q}_3^{(c)}(A_{2u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z75}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u},a) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} - \frac{\sqrt{3}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z76}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u},b) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} - \frac{\sqrt{3}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z77}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u},c) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z78}} \quad \mathbb{Q}_3^{(1,0;c)}(A_{2u}) = \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z79}} \quad \mathbb{Q}_3^{(1,1;c)}(A_{2u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

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

$$\boxed{\text{z81}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z82}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z83}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\begin{aligned}
\boxed{\text{z84}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, c) &= \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} + \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{7} \\
\boxed{\text{z85}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, c) &= -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} - \frac{\sqrt{21}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} \\
\boxed{\text{z143}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g) &= \frac{\sqrt{21}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} - \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} + \frac{2\sqrt{21}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} \\
\boxed{\text{z144}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g) &= -\frac{\sqrt{21}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{7} - \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{7} \\
\boxed{\text{z145}} \quad \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{z146}} \quad \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{z147}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g, b) &= \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} + \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{7} \\
\boxed{\text{z148}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, b) &= -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} - \frac{\sqrt{21}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} \\
\boxed{\text{z149}} \quad \mathbb{Q}_{4,1}^{(1,-1;c)}(E_g) &= \frac{\sqrt{21}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} - \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} + \frac{2\sqrt{21}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} \\
\boxed{\text{z150}} \quad \mathbb{Q}_{4,2}^{(1,-1;c)}(E_g) &= -\frac{\sqrt{21}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{7} - \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{7} \\
\boxed{\text{z151}} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g) &= \frac{\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{2} - \frac{\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{2} \\
\boxed{\text{z152}} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g) &= \frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} + \frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} - \frac{\sqrt{3}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} \\
\boxed{\text{z153}} \quad \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{z154}} \quad \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}
\end{aligned}$$

$$\begin{aligned}
\text{z155} \quad \mathbb{Q}_{5,1}^{(1,-1;c)}(E_u) &= \frac{\sqrt{70}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{28} - \frac{\sqrt{42}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{28} - \frac{\sqrt{70}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{28} - \frac{\sqrt{42}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{14} \\
\text{z156} \quad \mathbb{Q}_{5,2}^{(1,-1;c)}(E_u) &= \frac{\sqrt{210}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{84} + \frac{3\sqrt{14}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{28} + \frac{\sqrt{210}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{84} - \frac{3\sqrt{14}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{28} - \frac{\sqrt{210}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{42} \\
\text{z157} \quad \mathbb{G}_{2,1}^{(c)}(E_u, a) &= -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z158} \quad \mathbb{G}_{2,2}^{(c)}(E_u, a) &= \frac{\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z159} \quad \mathbb{G}_{2,1}^{(c)}(E_u, b) &= \frac{\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2} \\
\text{z160} \quad \mathbb{G}_{2,2}^{(c)}(E_u, b) &= \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\text{z161} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, a) &= -\frac{\sqrt{42}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{70}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{42}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} + \frac{\sqrt{70}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{14} \\
\text{z162} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, a) &= \frac{3\sqrt{14}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{210}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{84} - \frac{3\sqrt{14}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} - \frac{\sqrt{210}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{84} + \frac{\sqrt{210}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{42} \\
\text{z163} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, b) &= -\frac{3\sqrt{14}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{28} - \frac{\sqrt{210}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{84} + \frac{3\sqrt{14}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{28} \\
&\quad - \frac{\sqrt{210}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{84} + \frac{\sqrt{210}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{42} \\
\text{z164} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, b) &= -\frac{\sqrt{42}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{28} + \frac{\sqrt{70}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{28} - \frac{\sqrt{42}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{28} - \frac{\sqrt{70}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{14} \\
\text{z165} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, c) &= -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z166} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, c) &= \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z167} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E_u, d) &= \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2}
\end{aligned}$$

$$\begin{aligned}
\text{z168} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E_u, d) &= \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\text{z169} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(E_u) &= -\frac{\sqrt{210}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{84} + \frac{3\sqrt{14}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{210}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{84} - \frac{3\sqrt{14}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} + \frac{\sqrt{210}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{42} \\
\text{z233} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(E_u) &= \frac{\sqrt{70}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{28} - \frac{\sqrt{70}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{28} - \frac{\sqrt{42}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{14} \\
\text{z234} \quad \mathbb{G}_{2,1}^{(1,0;c)}(E_u, a) &= -\frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z235} \quad \mathbb{G}_{2,2}^{(1,0;c)}(E_u, a) &= -\frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z236} \quad \mathbb{G}_{2,1}^{(1,0;c)}(E_u, b) &= \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\sqrt{3}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{3}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\text{z237} \quad \mathbb{G}_{2,2}^{(1,0;c)}(E_u, b) &= -\frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2} \\
\text{z238} \quad \mathbb{G}_{2,1}^{(1,1;c)}(E_u, a) &= -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z239} \quad \mathbb{G}_{2,2}^{(1,1;c)}(E_u, a) &= \frac{\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\text{z240} \quad \mathbb{G}_{2,1}^{(1,1;c)}(E_u, b) &= \frac{\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} - \frac{\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2} \\
\text{z241} \quad \mathbb{G}_{2,2}^{(1,1;c)}(E_u, b) &= \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\text{z242} \quad \mathbb{Q}_{4,1}^{(c)}(T_{1g}) &= -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{4} - \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{12} \\
\text{z243} \quad \mathbb{Q}_{4,2}^{(c)}(T_{1g}) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{12} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} \\
\text{z244} \quad \mathbb{Q}_{4,3}^{(c)}(T_{1g}) &= \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}
\end{aligned}$$



$$\begin{aligned}
\boxed{\text{z245}} \quad \mathbb{Q}_{4,1}^{(1,-1;c)}(T_{1g}) &= -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{4} - \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{12} \\
\boxed{\text{z246}} \quad \mathbb{Q}_{4,2}^{(1,-1;c)}(T_{1g}) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{12} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} \\
\boxed{\text{z247}} \quad \mathbb{Q}_{4,3}^{(1,-1;c)}(T_{1g}) &= \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\boxed{\text{z248}} \quad \mathbb{G}_{1,1}^{(c)}(T_{1g}) &= -\frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} \\
\boxed{\text{z249}} \quad \mathbb{G}_{1,2}^{(c)}(T_{1g}) &= \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} - \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} \\
\boxed{\text{z250}} \quad \mathbb{G}_{1,3}^{(c)}(T_{1g}) &= -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{15} \\
\boxed{\text{z251}} \quad \mathbb{G}_{3,1}^{(c)}(T_{1g}) &= \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{20} - \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} - \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{60} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{60} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z252}} \quad \mathbb{G}_{3,2}^{(c)}(T_{1g}) &= -\frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{20} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{60} + \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{60} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z253}} \quad \mathbb{G}_{3,3}^{(c)}(T_{1g}) &= -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} \\
\boxed{\text{z254}} \quad \mathbb{G}_{1,1}^{(1,-1;c)}(T_{1g}) &= -\frac{\sqrt{10}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} \\
&\quad - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} \\
\boxed{\text{z255}} \quad \mathbb{G}_{1,2}^{(1,-1;c)}(T_{1g}) &= \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} \\
&\quad - \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} \\
\boxed{\text{z256}} \quad \mathbb{G}_{1,3}^{(1,-1;c)}(T_{1g}) &= -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{15}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z257}} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(T_{1g}) &= \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{20} - \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} - \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{60} \\
&+ \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{60} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z258}} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(T_{1g}) &= -\frac{\sqrt{10}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{20} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{60} \\
&+ \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{60} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z259}} \quad \mathbb{G}_{3,3}^{(1,-1;c)}(T_{1g}) &= -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} \\
\boxed{\text{z260}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(T_{1g}, a) &= \frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z261}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(T_{1g}, a) &= \frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z262}} \quad \mathbb{G}_{1,3}^{(1,0;c)}(T_{1g}, a) &= \frac{\sqrt{3}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z263}} \quad \mathbb{G}_{1,1}^{(1,0;c)}(T_{1g}, b) &= -\frac{\sqrt{30}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} + \frac{\sqrt{10}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{10}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} \\
\boxed{\text{z264}} \quad \mathbb{G}_{1,2}^{(1,0;c)}(T_{1g}, b) &= \frac{\sqrt{10}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{10} - \frac{\sqrt{30}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} - \frac{\sqrt{10}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{10}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} \\
\boxed{\text{z265}} \quad \mathbb{G}_{1,3}^{(1,0;c)}(T_{1g}, b) &= \frac{\sqrt{10}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} + \frac{\sqrt{30}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{15} \\
\boxed{\text{z266}} \quad \mathbb{G}_{3,1}^{(1,0;c)}(T_{1g}) &= -\frac{\sqrt{5}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} - \frac{\sqrt{15}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z267}} \quad \mathbb{G}_{3,2}^{(1,0;c)}(T_{1g}) &= -\frac{\sqrt{15}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} - \frac{\sqrt{5}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{15}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z268}} \quad \mathbb{G}_{3,3}^{(1,0;c)}(T_{1g}) &= -\frac{\sqrt{15}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{15}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{5}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z281}} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}, a) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z282}} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}, a) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z283}} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}, a) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z284}} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z285}} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z286}} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z294}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}, a) &= -\frac{\sqrt{21}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{21} - \frac{\sqrt{35}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{21} - \frac{\sqrt{21}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{21} + \frac{\sqrt{35}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{21} + \frac{\sqrt{35}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{21} \\
\boxed{\text{z295}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}, a) &= -\frac{\sqrt{21}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{21} + \frac{\sqrt{35}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{21} - \frac{\sqrt{21}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{21} - \frac{\sqrt{35}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{21} + \frac{\sqrt{35}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{21} \\
\boxed{\text{z296}} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}, a) &= -\frac{\sqrt{21}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{21} - \frac{\sqrt{35}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{21} - \frac{\sqrt{21}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{21} + \frac{\sqrt{35}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{21} + \frac{\sqrt{35}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{21} \\
\boxed{\text{z297}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z298}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}, b) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z299}} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z338}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(T_{1u}, c) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z339}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(T_{1u}, c) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}
\end{aligned}$$

$$\begin{aligned}
\text{z340} \quad \mathbb{Q}_{1,3}^{(1,-1;c)}(T_{1u}, c) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z341} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{1u}, a) &= -\frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} \\
\text{z342} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{1u}, a) &= \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} \\
\text{z343} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{1u}, a) &= -\frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} \\
\text{z344} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{1u}, b) &= -\frac{\sqrt{105}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{84} - \frac{5\sqrt{7}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{84} - \frac{\sqrt{105}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{84} \\
&\quad + \frac{5\sqrt{7}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{84} - \frac{4\sqrt{7}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{21} \\
\text{z345} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{1u}, b) &= -\frac{\sqrt{105}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{84} + \frac{5\sqrt{7}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{84} - \frac{\sqrt{105}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{84} \\
&\quad - \frac{5\sqrt{7}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{84} - \frac{4\sqrt{7}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{21} \\
\text{z346} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{1u}, b) &= -\frac{\sqrt{105}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{84} - \frac{5\sqrt{7}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{84} - \frac{\sqrt{105}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{84} \\
&\quad + \frac{5\sqrt{7}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{84} - \frac{4\sqrt{7}\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{21} \\
\text{z347} \quad \mathbb{Q}_{5,1}^{(1,-1;c)}(T_{1u}, 2) &= \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{12} - \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{4} + \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{12} + \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{4} \\
\text{z348} \quad \mathbb{Q}_{5,2}^{(1,-1;c)}(T_{1u}, 2) &= \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{12} + \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{4} + \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{4} \\
\text{z349} \quad \mathbb{Q}_{5,3}^{(1,-1;c)}(T_{1u}, 2) &= \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{12} - \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{4} + \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{12} + \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{4} \\
\text{z350} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(T_{1u}, a) &= -\frac{\sqrt{30}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{30} + \frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10}
\end{aligned}$$

$$\begin{aligned}
\text{z351} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(T_{1u}, a) &= -\frac{\sqrt{30}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{30} + \frac{\sqrt{10}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{10} - \frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} \\
\text{z352} \quad \mathbb{Q}_{1,3}^{(1,0;c)}(T_{1u}, a) &= \frac{\sqrt{30}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} + \frac{\sqrt{10}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} + \frac{\sqrt{10}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} \\
\text{z353} \quad \mathbb{Q}_{1,1}^{(1,0;c)}(T_{1u}, b) &= -\frac{\sqrt{6}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} - \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} - \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{2}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\text{z354} \quad \mathbb{Q}_{1,2}^{(1,0;c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{2}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z355} \quad \mathbb{Q}_{1,3}^{(1,0;c)}(T_{1u}, b) &= -\frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z356} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{1u}, a) &= -\frac{\sqrt{5}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} + \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{15} \\
\text{z357} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{1u}, a) &= -\frac{\sqrt{5}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{10} - \frac{\sqrt{15}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{15} \\
\text{z358} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{1u}, a) &= \frac{\sqrt{5}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{5} - \frac{\sqrt{15}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{15} - \frac{\sqrt{15}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{15} \\
\text{z359} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{1u}, b) &= \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} + \frac{\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} \\
\text{z360} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{1u}, b) &= -\frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} \\
\text{z361} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{1u}, b) &= -\frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} \\
\text{z440} \quad \mathbb{Q}_{1,1}^{(1,1;c)}(T_{1u}, a) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\text{z441} \quad \mathbb{Q}_{1,2}^{(1,1;c)}(T_{1u}, a) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\text{z442} \quad \mathbb{Q}_{1,3}^{(1,1;c)}(T_{1u}, a) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}
\end{aligned}$$

$$\boxed{\text{z443}} \quad \mathbb{Q}_{1,1}^{(1,1;c)}(T_{1u}, b) = \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z444}} \quad \mathbb{Q}_{1,2}^{(1,1;c)}(T_{1u}, b) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z445}} \quad \mathbb{Q}_{1,3}^{(1,1;c)}(T_{1u}, b) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z446}} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(T_{1u}) = \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{4}$$

$$\boxed{\text{z447}} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(T_{1u}) = -\frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{4} + \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{4}$$

$$\boxed{\text{z448}} \quad \mathbb{G}_{4,3}^{(1,-1;c)}(T_{1u}) = \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{4} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{4}$$

$$\boxed{\text{z449}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, a) = \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3}$$

$$\boxed{\text{z450}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, a) = \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3}$$

$$\boxed{\text{z451}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, a) = \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3}$$

$$\boxed{\text{z452}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, b) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z453}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, b) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z454}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, b) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z455}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, c) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{42} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} - \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} - \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14}$$

$$\boxed{\text{z456}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, c) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{42} + \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14}$$

$$\begin{aligned}
\text{z457} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, c) &= -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} + \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} \\
\text{z458} \quad \mathbb{Q}_{4,1}^{(c)}(T_{2g}) &= -\frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{28} - \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} + \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} \\
\text{z459} \quad \mathbb{Q}_{4,2}^{(c)}(T_{2g}) &= -\frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{28} - \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} \\
\text{z460} \quad \mathbb{Q}_{4,3}^{(c)}(T_{2g}) &= \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} \\
\text{z461} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z462} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z463} \quad \mathbb{Q}_{2,3}^{(1,-1;c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\text{z464} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(T_{2g}, b) &= \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{42} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} - \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} \\
&\quad - \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} \\
\text{z465} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(T_{2g}, b) &= \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{42} + \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} \\
&\quad + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} \\
\text{z466} \quad \mathbb{Q}_{2,3}^{(1,-1;c)}(T_{2g}, b) &= -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} + \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} \\
\text{z467} \quad \mathbb{Q}_{4,1}^{(1,-1;c)}(T_{2g}) &= -\frac{\sqrt{14}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{28} - \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} \\
&\quad + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} + \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21}
\end{aligned}$$

$$\begin{aligned}
\text{z468} \quad \mathbb{Q}_{4,2}^{(1,-1;c)}(T_{2g}) &= -\frac{\sqrt{14}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{28} \\
&\quad - \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} \\
\text{z469} \quad \mathbb{Q}_{4,3}^{(1,-1;c)}(T_{2g}) &= \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} \\
\text{z470} \quad \mathbb{Q}_{2,1}^{(1,0;c)}(T_{2g}) &= -\frac{\sqrt{6}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} \\
\text{z471} \quad \mathbb{Q}_{2,2}^{(1,0;c)}(T_{2g}) &= \frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{2}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} \\
\text{z472} \quad \mathbb{Q}_{2,3}^{(1,0;c)}(T_{2g}) &= -\frac{\sqrt{2}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{6} + \frac{\sqrt{2}\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\text{z473} \quad \mathbb{Q}_{2,1}^{(1,1;c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} \\
\text{z474} \quad \mathbb{Q}_{2,2}^{(1,1;c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} \\
\text{z475} \quad \mathbb{Q}_{2,3}^{(1,1;c)}(T_{2g}) &= \frac{\sqrt{3}\mathbb{Q}_0^{(1,1;a)}(A_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} \\
\text{z476} \quad \mathbb{G}_{3,1}^{(c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{12} - \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{4} \\
\text{z477} \quad \mathbb{G}_{3,2}^{(c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{12} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} \\
\text{z478} \quad \mathbb{G}_{3,3}^{(c)}(T_{2g}) &= -\frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} \\
\text{z479} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{12} - \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{4} \\
\text{z480} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{12} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4}
\end{aligned}$$



$$\begin{aligned}
\text{z481} \quad \mathbb{G}_{3,3}^{(1,-1;c)}(T_{2g}) &= -\frac{\sqrt{6}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} \\
\text{z482} \quad \mathbb{G}_{3,1}^{(1,0;c)}(T_{2g}) &= -\frac{\sqrt{3}\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} - \frac{\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} \\
\text{z483} \quad \mathbb{G}_{3,2}^{(1,0;c)}(T_{2g}) &= -\frac{\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} + \frac{\sqrt{3}\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} \\
\text{z484} \quad \mathbb{G}_{3,3}^{(1,0;c)}(T_{2g}) &= \frac{\mathbb{G}_{1,1}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} - \frac{\mathbb{G}_{1,2}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3} + \frac{\mathbb{G}_{1,3}^{(1,0;a)}(T_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\text{z560} \quad \mathbb{Q}_{3,1}^{(c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\text{z561} \quad \mathbb{Q}_{3,2}^{(c)}(T_{2u}) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z562} \quad \mathbb{Q}_{3,3}^{(c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z563} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{2u},a) &= \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\text{z564} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{2u},a) &= \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} \\
\text{z565} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{2u},a) &= \frac{\sqrt{15}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} - \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{12} + \frac{\mathbb{M}_3^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\text{z566} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{2u},b) &= \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{24} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{24} - \frac{\sqrt{10}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{8} \\
\text{z567} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{2u},b) &= -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{24} - \frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{8} + \frac{\sqrt{6}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{24} - \frac{\sqrt{10}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{8} \\
\text{z568} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{2u},b) &= \frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{24} - \frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{24} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{8} \\
\text{z569} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(T_{2u},c) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6}
\end{aligned}$$

$$\begin{aligned}
\text{z570} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(T_{2u}, c) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z571} \quad \mathbb{Q}_{3,3}^{(1,-1;c)}(T_{2u}, c) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z572} \quad \mathbb{Q}_{5,1}^{(1,-1;c)}(T_{2u}) &= -\frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{24} + \frac{\sqrt{10}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{24} \\
\text{z573} \quad \mathbb{Q}_{5,2}^{(1,-1;c)}(T_{2u}) &= \frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{24} - \frac{\sqrt{10}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,3}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{24} \\
\text{z574} \quad \mathbb{Q}_{5,3}^{(1,-1;c)}(T_{2u}) &= -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{24} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{24} \\
\text{z575} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{2u}, a) &= -\frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} \\
\text{z576} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{2u}, a) &= \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\text{z577} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{2u}, a) &= -\frac{\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} \\
\text{z578} \quad \mathbb{Q}_{3,1}^{(1,0;c)}(T_{2u}, b) &= \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} - \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} \\
\text{z579} \quad \mathbb{Q}_{3,2}^{(1,0;c)}(T_{2u}, b) &= \frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2} \\
\text{z580} \quad \mathbb{Q}_{3,3}^{(1,0;c)}(T_{2u}, b) &= -\frac{\sqrt{3}\mathbb{T}_{2,1}^{(1,0;a)}(E_g)\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3} \\
\text{z581} \quad \mathbb{Q}_{3,1}^{(1,1;c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\text{z582} \quad \mathbb{Q}_{3,2}^{(1,1;c)}(T_{2u}) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\text{z583} \quad \mathbb{Q}_{3,3}^{(1,1;c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}
\end{aligned}$$



$$\boxed{\text{z598}} \quad \mathbb{G}_{2,3}^{(1,0;c)}(T_{2u}, a) = -\frac{\sqrt{2}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(E_g)\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} + \frac{\sqrt{2}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z599}} \quad \mathbb{G}_{2,1}^{(1,0;c)}(T_{2u}, b) = \frac{\sqrt{6}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z600}} \quad \mathbb{G}_{2,2}^{(1,0;c)}(T_{2u}, b) = \frac{\sqrt{6}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{2,3}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z601}} \quad \mathbb{G}_{2,3}^{(1,0;c)}(T_{2u}, b) = \frac{\sqrt{6}\mathbb{T}_{2,1}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{T}_{2,2}^{(1,0;a)}(T_{2g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$$\boxed{\text{z602}} \quad \mathbb{G}_{2,1}^{(1,1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z603}} \quad \mathbb{G}_{2,2}^{(1,1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z604}} \quad \mathbb{G}_{2,3}^{(1,1;c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,1;a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

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## Atomic SAMB

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

$$\boxed{\text{x1}} \quad \mathbb{Q}_0^{(a)}(A_{1g}) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$$

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

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

$$\boxed{\text{x4}} \quad \mathbb{M}_{1,3}^{(1,-1;a)}(T_{1g}) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{bmatrix}$$

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

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

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

$$\boxed{\text{x7}} \quad \mathbb{Q}_{1,3}^{(a)}(T_{1u}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

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

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

$$\boxed{\text{x10}} \quad \mathbb{Q}_{1,3}^{(1,0;a)}(T_{1u}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x11}} \quad \mathbb{G}_{2,1}^{(1,-1;a)}(E_u) = \begin{bmatrix} 0 & -\frac{\sqrt{6}i}{12} & 0 & -\frac{\sqrt{6}}{12} & \frac{\sqrt{6}i}{6} & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}i}{6} \end{bmatrix}$$

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

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

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

$$\boxed{\text{x15}} \quad \mathbb{G}_{2,3}^{(1,-1;a)}(T_{2u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$$

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

$$\boxed{\text{x17}} \quad \mathbb{M}_{2,1}^{(1,-1;a)}(E_u) = \begin{bmatrix} 0 & -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}}{6} & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{6}}{6} \end{bmatrix}$$

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

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

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

$$\boxed{\text{x21}} \quad \mathbb{M}_{2,3}^{(1,-1;a)}(T_{2u}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

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

$$\boxed{\text{x23}} \quad \mathbb{T}_{1,1}^{(a)}(T_{1u}) = \begin{bmatrix} \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

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

$$\boxed{\text{x25}} \quad \mathbb{T}_{1,3}^{(a)}(T_{1u}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} \end{bmatrix}$$

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

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

$$\boxed{\text{x28}} \quad \mathbb{T}_{1,3}^{(1,0;a)}(T_{1u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

• 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:  $|p_x, \uparrow\rangle, |p_x, \downarrow\rangle, |p_y, \uparrow\rangle, |p_y, \downarrow\rangle, |p_z, \uparrow\rangle, |p_z, \downarrow\rangle$

$$\boxed{\text{x29}} \quad \mathbb{Q}_0^{(a)}(A_{1g}) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \end{bmatrix}$$

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

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

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

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

$$\boxed{\text{x34}} \quad \mathbb{Q}_{2,3}^{(a)}(T_{2g}) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

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

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

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

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

$$\boxed{\text{x39}} \quad \mathbb{Q}_{2,3}^{(1,-1;a)}(T_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$



$$\boxed{\text{x40}} \quad \mathbb{Q}_0^{(1,1;a)}(A_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{\text{x43}} \quad \mathbb{G}_{1,3}^{(1,0;a)}(T_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{\text{x46}} \quad \mathbb{M}_{1,3}^{(a)}(T_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x47}} \quad \mathbb{M}_3^{(1,-1;a)}(A_{2g}) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x48}} \quad \mathbb{M}_{1,1}^{(1,-1;a)}(T_{1g}) = \begin{bmatrix} 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \end{bmatrix}$$

$$\boxed{\text{x49}} \quad \mathbb{M}_{1,2}^{(1,-1;a)}(T_{1g}) = \begin{bmatrix} 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$$

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

$$\boxed{\text{x51}} \quad \mathbb{M}_{3,1}^{(1,-1;a)}(T_{1g}) = \begin{bmatrix} 0 & \frac{\sqrt{5}}{5} & 0 & \frac{\sqrt{5}i}{10} & -\frac{\sqrt{5}}{10} & 0 \\ \frac{\sqrt{5}}{5} & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & \frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 \\ -\frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 \end{bmatrix}$$

$$\boxed{\text{x52}} \quad \mathbb{M}_{3,2}^{(1,-1;a)}(T_{1g}) = \begin{bmatrix} 0 & \frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 \\ -\frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{5}}{10} & 0 & -\frac{\sqrt{5}i}{5} & -\frac{\sqrt{5}}{10} & 0 \\ -\frac{\sqrt{5}}{10} & 0 & \frac{\sqrt{5}i}{5} & 0 & 0 & \frac{\sqrt{5}}{10} \\ 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & \frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{5}}{10} & -\frac{\sqrt{5}i}{10} & 0 \end{bmatrix}$$

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

$$\boxed{\text{x54}} \quad \mathbb{M}_{3,1}^{(1,-1;a)}(T_{2g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} \\ 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \end{bmatrix}$$

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

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

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

$$\boxed{\text{x58}} \quad \mathbb{M}_{1,2}^{(1,1;a)}(T_{1g}) = \begin{bmatrix} 0 & \frac{\sqrt{30}i}{30} & 0 & \frac{\sqrt{30}}{20} & 0 & 0 \\ -\frac{\sqrt{30}i}{30} & 0 & \frac{\sqrt{30}}{20} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{15} & \frac{\sqrt{30}}{20} & 0 \\ \frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{15} & 0 & 0 & -\frac{\sqrt{30}}{20} \\ 0 & 0 & \frac{\sqrt{30}}{20} & 0 & 0 & \frac{\sqrt{30}i}{30} \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{20} & -\frac{\sqrt{30}i}{30} & 0 \end{bmatrix}$$

$$\boxed{\text{x59}} \quad \mathbb{M}_{1,3}^{(1,1;a)}(T_{1g}) = \begin{bmatrix} -\frac{\sqrt{30}}{30} & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{20} \\ 0 & \frac{\sqrt{30}}{30} & 0 & 0 & \frac{\sqrt{30}}{20} & 0 \\ 0 & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 & -\frac{\sqrt{30}i}{20} \\ 0 & 0 & 0 & \frac{\sqrt{30}}{30} & \frac{\sqrt{30}i}{20} & 0 \\ 0 & \frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{20} & \frac{\sqrt{30}}{15} & 0 \\ \frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{20} & 0 & 0 & -\frac{\sqrt{30}}{15} \end{bmatrix}$$

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

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

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

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

$$\boxed{\text{x64}} \quad \mathbb{T}_{2,3}^{(1,0;a)}(T_{2g}) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ 0 & -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{bmatrix}$$

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## Cluster SAMB

- Site cluster

\*\* Wyckoff: 1a

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

- Bond cluster

\*\* Wyckoff: 3a@3d

$$\boxed{\text{y2}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3} \right]$$

$$\boxed{\text{y3}} \quad \mathbb{Q}_{2,1}^{(s)}(E_g) = \left[ -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{3} \right]$$

$$\boxed{\text{y4}} \quad \mathbb{Q}_{2,2}^{(s)}(E_g) = \left[ \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}, 0 \right]$$

$$\boxed{\text{y5}} \quad \mathbb{T}_{1,1}^{(s)}(T_{1u}) = [i, 0, 0]$$

$$\boxed{\text{y6}} \quad \mathbb{T}_{1,2}^{(s)}(T_{1u}) = [0, i, 0]$$

$$\boxed{\text{y7}} \quad \mathbb{T}_{1,3}^{(s)}(T_{1u}) = [0, 0, i]$$

\*\* Wyckoff: 6b@3c

$$\boxed{\text{y8}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y9}} \quad \mathbb{Q}_{2,1}^{(s)}(E_g) = \left[ -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3} \right]$$

$$\boxed{\text{y10}} \quad \mathbb{Q}_{2,2}^{(s)}(E_g) = \left[ \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, 0, 0 \right]$$

$$\boxed{\text{y11}} \quad \mathbb{T}_{1,1}^{(s)}(T_{1u}) = \left[ 0, 0, \frac{i}{2}, \frac{i}{2}, \frac{i}{2}, -\frac{i}{2} \right]$$

$$\boxed{\text{y12}} \quad \mathbb{T}_{1,2}^{(s)}(T_{1u}) = \left[ \frac{i}{2}, -\frac{i}{2}, 0, 0, \frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{\text{y13}} \quad \mathbb{T}_{1,3}^{(s)}(T_{1u}) = \left[ \frac{i}{2}, \frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, 0, 0 \right]$$

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

$$\boxed{\text{y15}} \quad \mathbb{Q}_{2,2}^{(s)}(T_{2g}) = \left[ 0, 0, \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}, 0, 0 \right]$$

$$\boxed{\text{y16}} \quad \mathbb{Q}_{2,3}^{(s)}(T_{2g}) = \left[ 0, 0, 0, 0, \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

$$\boxed{\text{y17}} \quad \mathbb{M}_{2,1}^{(s)}(T_{2u}) = \left[ 0, 0, \frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, \frac{i}{2} \right]$$

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

$$\boxed{\text{y19}} \quad \mathbb{M}_{2,3}^{(s)}(T_{2u}) = \left[ \frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, \frac{i}{2}, 0, 0 \right]$$

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**Site and Bond**


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Table 5: Orbital of each site

| # | site     | orbital  |
|---|----------|--|
| 1 | <b>A</b> | $ s, \uparrow\rangle,  s, \downarrow\rangle,  p_x, \uparrow\rangle,  p_x, \downarrow\rangle,  p_y, \uparrow\rangle,  p_y, \downarrow\rangle,  p_z, \uparrow\rangle,  p_z, \downarrow\rangle$ |

Table 6: Neighbor and bra-ket of each bond

| # | head     | tail     | neighbor | head (bra) | tail (ket) |
|---|----------|----------|----------|------------|------------|
| 1 | <b>A</b> | <b>A</b> | [1,2]    | [s,p]      | [s,p]      |

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**Site in Unit Cell**


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

Table 7: 'A' (#1) site cluster (1a), m-3m

| SL | position ( $\mathbf{s}$ )    | mapping          |
|----|------------------------------|------------------|
| 1  | [ 0.00000, 0.00000, 0.00000] | [1,2,3,4,...,48] |

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**Bond in Unit Cell**


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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 (3a@3d), ND,  $|\mathbf{v}|=1.0$  (cartesian)

| SL | vector ( $\mathbf{v}$ )      | center ( $\mathbf{c}$ )      | mapping  | head  | tail  | $\mathbf{R}$ (primitive) |
|----|------------------------------|------------------------------|--|-------|-------|--------------------------|
| 1  | [-1.00000, 0.00000, 0.00000] | [ 0.50000, 0.00000, 0.00000] | [1,-2,-3,4,17,-18,-19,20,-25,26,27,-28,-41,42,43,-44]    | (1,1) | (1,1) | [1,0,0]                  |
| 2  | [ 0.00000,-1.00000, 0.00000] | [ 0.00000, 0.50000, 0.00000] | [5,-6,-7,8,13,-14,-15,16,-29,30,31,-32,-37,38,39,-40]    | (1,1) | (1,1) | [0,1,0]                  |
| 3  | [ 0.00000, 0.00000,-1.00000] | [ 0.00000, 0.00000, 0.50000] | [9,-10,-11,12,-21,22,23,-24,-33,34,35,-36,45,-46,-47,48] | (1,1) | (1,1) | [0,0,1]                  |



Table 9: 2-th 'A'-'A' [1] (#2) bond cluster (6b03c), ND,  $|\mathbf{v}|= 1.41421$  (cartesian)

| SL | vector ( $\mathbf{v}$ )        | center ( $\mathbf{c}$ )      | mapping                              | head   | tail   | $\mathbf{R}$ (primitive) |
|----|--------------------------------|------------------------------|--------------------------------------|--------|--------|--------------------------|
| 1  | [ 0.00000, -1.00000, -1.00000] | [ 0.00000, 0.50000, 0.50000] | [1, -4, 18, -19, -25, 28, -42, 43]   | (1, 1) | (1, 1) | [0, 1, 1]                |
| 2  | [ 0.00000, 1.00000, -1.00000]  | [ 0.00000, 0.50000, 0.50000] | [2, -3, -17, 20, -26, 27, 41, -44]   | (1, 1) | (1, 1) | [0, -1, 1]               |
| 3  | [-1.00000, 0.00000, -1.00000]  | [ 0.50000, 0.00000, 0.50000] | [5, -8, -14, 15, -29, 32, 38, -39]   | (1, 1) | (1, 1) | [1, 0, 1]                |
| 4  | [-1.00000, 0.00000, 1.00000]   | [ 0.50000, 0.00000, 0.50000] | [6, -7, 13, -16, -30, 31, -37, 40]   | (1, 1) | (1, 1) | [1, 0, -1]               |
| 5  | [-1.00000, -1.00000, 0.00000]  | [ 0.50000, 0.50000, 0.00000] | [9, -12, 21, -24, -33, 36, -45, 48]  | (1, 1) | (1, 1) | [1, 1, 0]                |
| 6  | [ 1.00000, -1.00000, 0.00000]  | [ 0.50000, 0.50000, 0.00000] | [10, -11, -22, 23, -34, 35, 46, -47] | (1, 1) | (1, 1) | [-1, 1, 0]               |