

Model for “Mn3Sn”

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General Condition

- Basis type: 1g
- SAMB selection:
 - Type: [Q, G]
 - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
 - Irrep.: [A_{1g}, A_{2g}, B_{1g}, B_{2g}, E_{1g}, E_{2g}, A_{1u}, A_{2u}, B_{1u}, B_{2u}, E_{1u}, E_{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}, B_{1g}, B_{2g}, E_{1g}, E_{2g}, A_{1u}, A_{2u}, B_{1u}, B_{2u}, E_{1u}, E_{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}, B_{1g}, B_{2g}, E_{1g}, E_{2g}, A_{1u}, A_{2u}, B_{1u}, B_{2u}, E_{1u}, E_{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}, B_{1g}, B_{2g}, E_{1g}, E_{2g}, A_{1u}, A_{2u}, B_{1u}, B_{2u}, E_{1u}, E_{2u}]
- Max. neighbor: 10
- Search cell range: (-2, 3), (-2, 3), (-2, 3)
- Toroidal priority: false

Group and Unit Cell

- Group: SG No. 194 D_{6h}⁴ P6₃/mmc [hexagonal]
- Associated point group: PG No. 194 D_{6h} 6/mmm [hexagonal]
- Unit cell:

a = 1.00000, b = 1.00000, c = 1.00000, α = 90.0, β = 90.0, γ = 120.0
- Lattice vectors (conventional cell):

a_1 = [1.00000, 0.00000, 0.00000]
 a_2 = [-0.50000, 0.86603, 0.00000]
 a_3 = [0.00000, 0.00000, 1.00000]

Symmetry Operation

Table 1: Symmetry operation

| # | SO | # | SO | # | SO | # | SO | # | SO |
|----|--|----|---|----|---|----|---|----|--|
| 1 | {1 0} | 2 | {3 ⁺ ₀₀₁ 0} | 3 | {3 ⁻ ₀₀₁ 0} | 4 | {2 ₀₀₁ 00 ¹ ₂ } | 5 | {6 ⁻ ₀₀₁ 00 ¹ ₂ } |
| 6 | {6 ⁺ ₀₀₁ 00 ¹ ₂ } | 7 | {2 ₁₁₀ 0} | 8 | {2 ₁₀₀ 0} | 9 | {2 ₀₁₀ 0} | 10 | {2 ₁₋₁₀ 00 ¹ ₂ } |
| 11 | {2 ₁₂₀ 00 ¹ ₂ } | 12 | {2 ₂₁₀ 00 ¹ ₂ } | 13 | {-1 0} | 14 | {-3 ⁺ ₀₀₁ 0} | 15 | {-3 ⁻ ₀₀₁ 0} |
| 16 | {m ₀₀₁ 00 ¹ ₂ } | 17 | {-6 ⁻ ₀₀₁ 00 ¹ ₂ } | 18 | {-6 ⁺ ₀₀₁ 00 ¹ ₂ } | 19 | {m ₁₁₀ 0} | 20 | {m ₁₀₀ 0} |
| 21 | {m ₀₁₀ 0} | 22 | {m ₁₋₁₀ 00 ¹ ₂ } | 23 | {m ₁₂₀ 00 ¹ ₂ } | 24 | {m ₂₁₀ 00 ¹ ₂ } | | |

Harmonics

Table 2: Harmonics

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|---|---------------------------|----------|------|--------|--------------|-----------|---|
| 1 | $\mathbb{Q}_0(A_{1g})$ | A_{1g} | 0 | Q, T | - | - | 1 |
| 2 | $\mathbb{Q}_2(A_{1g})$ | A_{1g} | 2 | Q, T | - | - | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| 3 | $\mathbb{Q}_4(A_{1g})$ | A_{1g} | 4 | Q, T | - | - | $\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$ |
| 4 | $\mathbb{Q}_6(A_{1g}, 2)$ | A_{1g} | 6 | Q, T | 2 | - | $\frac{\sqrt{462}(x-y)(x+y)(x^2-4xy+y^2)(x^2+4xy+y^2)}{32}$ |
| 5 | $\mathbb{G}_0(A_{1u})$ | A_{1u} | 0 | G, M | - | - | 1 |
| 6 | $\mathbb{G}_2(A_{1u})$ | A_{1u} | 2 | G, M | - | - | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |

continued ...

Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|----|---------------------------|----------|------|--------|--------------|-----------|---|
| 7 | $\mathbb{G}_4(A_{1u})$ | A_{1u} | 4 | G, M | - | - | $\frac{3x^4}{8} + \frac{3x^2y^2}{4} - 3x^2z^2 + \frac{3y^4}{8} - 3y^2z^2 + z^4$ |
| 8 | $\mathbb{G}_6(A_{1u}, 2)$ | A_{1u} | 6 | G, M | 2 | - | $\frac{\sqrt{462}(x-y)(x+y)(x^2-4xy+y^2)(x^2+4xy+y^2)}{32}$ |
| 9 | $\mathbb{Q}_7(A_{1u})$ | A_{1u} | 7 | Q, T | - | - | $\frac{\sqrt{6006xyz(x^2-3y^2)(3x^2-y^2)}}{16}$ |
| 10 | $\mathbb{G}_1(A_{2g})$ | A_{2g} | 1 | G, M | - | - | z |
| 11 | $\mathbb{G}_3(A_{2g})$ | A_{2g} | 3 | G, M | - | - | $-\frac{z(3x^2+3y^2-2z^2)}{2}$ |
| 12 | $\mathbb{G}_5(A_{2g})$ | A_{2g} | 5 | G, M | - | - | $\frac{z(15x^4+30x^2y^2-40x^2z^2+15y^4-40y^2z^2+8z^4)}{8}$ |
| 13 | $\mathbb{Q}_6(A_{2g})$ | A_{2g} | 6 | Q, T | - | - | $\frac{\sqrt{462xy(x^2-3y^2)(3x^2-y^2)}}{16}$ |
| 14 | $\mathbb{Q}_1(A_{2u})$ | A_{2u} | 1 | Q, T | - | - | z |
| 15 | $\mathbb{Q}_3(A_{2u})$ | A_{2u} | 3 | Q, T | - | - | $-\frac{z(3x^2+3y^2-2z^2)}{2}$ |
| 16 | $\mathbb{G}_6(A_{2u})$ | A_{2u} | 6 | G, M | - | - | $\frac{\sqrt{462xy(x^2-3y^2)(3x^2-y^2)}}{16}$ |
| 17 | $\mathbb{Q}_7(A_{2u}, 2)$ | A_{2u} | 7 | Q, T | 2 | - | $\frac{\sqrt{6006z(x-y)(x+y)(x^2-4xy+y^2)(x^2+4xy+y^2)}}{32}$ |
| 18 | $\mathbb{G}_3(B_{1g})$ | B_{1g} | 3 | G, M | - | - | $\frac{\sqrt{10y(3x^2-y^2)}}{4}$ |
| 19 | $\mathbb{Q}_4(B_{1g})$ | B_{1g} | 4 | Q, T | - | - | $\frac{\sqrt{70xz(x^2-3y^2)}}{4}$ |
| 20 | $\mathbb{Q}_6(B_{1g})$ | B_{1g} | 6 | Q, T | - | - | $-\frac{\sqrt{210xz(x^2-3y^2)(3x^2+3y^2-8z^2)}}{16}$ |
| 21 | $\mathbb{Q}_3(B_{1u})$ | B_{1u} | 3 | Q, T | - | - | $\frac{\sqrt{10y(3x^2-y^2)}}{4}$ |
| 22 | $\mathbb{G}_4(B_{1u})$ | B_{1u} | 4 | G, M | - | - | $\frac{\sqrt{70xz(x^2-3y^2)}}{4}$ |
| 23 | $\mathbb{Q}_5(B_{1u})$ | B_{1u} | 5 | Q, T | - | - | $-\frac{\sqrt{70y(3x^2-y^2)(x^2+y^2-8z^2)}}{16}$ |
| 24 | $\mathbb{Q}_9(B_{1u}, 1)$ | B_{1u} | 9 | Q, T | 1 | - | $\frac{\sqrt{24310y(3x^2-y^2)(3x^6-27x^4y^2+33x^2y^4-y^6)}}{256}$ |
| 25 | $\mathbb{G}_3(B_{2g})$ | B_{2g} | 3 | G, M | - | - | $\frac{\sqrt{10x(x^2-3y^2)}}{4}$ |
| 26 | $\mathbb{Q}_4(B_{2g})$ | B_{2g} | 4 | Q, T | - | - | $\frac{\sqrt{70yz(3x^2-y^2)}}{4}$ |
| 27 | $\mathbb{Q}_6(B_{2g})$ | B_{2g} | 6 | Q, T | - | - | $-\frac{\sqrt{210yz(3x^2-y^2)(3x^2+3y^2-8z^2)}}{16}$ |

continued ...

Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|----|-------------------------------|----------|------|--------|--------------|-----------|---|
| 28 | $\mathbb{Q}_3(B_{2u})$ | B_{2u} | 3 | Q, T | - | - | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$ |
| 29 | $\mathbb{G}_4(B_{2u})$ | B_{2u} | 4 | G, M | - | - | $\frac{\sqrt{70}yz(3x^2-y^2)}{4}$ |
| 30 | $\mathbb{Q}_5(B_{2u})$ | B_{2u} | 5 | Q, T | - | - | $-\frac{\sqrt{70}x(x^2-3y^2)(x^2+y^2-8z^2)}{16}$ |
| 31 | $\mathbb{Q}_9(B_{2u}, 1)$ | B_{2u} | 9 | Q, T | 1 | - | $\frac{\sqrt{24310}x(x^2-3y^2)(x^6-33x^4y^2+27x^2y^4-3y^6)}{256}$ |
| 32 | $\mathbb{G}_{1,1}(E_{1g})$ | E_{1g} | 1 | G, M | - | 1 | x |
| 33 | $\mathbb{G}_{1,2}(E_{1g})$ | | | | | 2 | y |
| 34 | $\mathbb{Q}_{2,1}(E_{1g})$ | E_{1g} | 2 | Q, T | - | 1 | $\sqrt{3}yz$ |
| 35 | $\mathbb{Q}_{2,2}(E_{1g})$ | | | | | 2 | $-\sqrt{3}xz$ |
| 36 | $\mathbb{G}_{3,1}(E_{1g})$ | E_{1g} | 3 | G, M | - | 1 | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$ |
| 37 | $\mathbb{G}_{3,2}(E_{1g})$ | | | | | 2 | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$ |
| 38 | $\mathbb{Q}_{4,1}(E_{1g})$ | E_{1g} | 4 | Q, T | - | 1 | $-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$ |
| 39 | $\mathbb{Q}_{4,2}(E_{1g})$ | | | | | 2 | $\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$ |
| 40 | $\mathbb{G}_{5,1}(E_{1g}, 1)$ | E_{1g} | 5 | G, M | 1 | 1 | $\frac{3\sqrt{14}x(x^4-10x^2y^2+5y^4)}{16}$ |
| 41 | $\mathbb{G}_{5,2}(E_{1g}, 1)$ | | | | | 2 | $-\frac{3\sqrt{14}y(5x^4-10x^2y^2+y^4)}{16}$ |
| 42 | $\mathbb{Q}_{6,1}(E_{1g}, 1)$ | E_{1g} | 6 | Q, T | 1 | 1 | $\frac{3\sqrt{154}yz(5x^4-10x^2y^2+y^4)}{16}$ |
| 43 | $\mathbb{Q}_{6,2}(E_{1g}, 1)$ | | | | | 2 | $\frac{3\sqrt{154}xz(x^4-10x^2y^2+5y^4)}{16}$ |
| 44 | $\mathbb{Q}_{6,1}(E_{1g}, 2)$ | E_{1g} | 6 | Q, T | 2 | 1 | $\frac{\sqrt{21}yz(5x^4+10x^2y^2-20x^2z^2+5y^4-20y^2z^2+8z^4)}{8}$ |
| 45 | $\mathbb{Q}_{6,2}(E_{1g}, 2)$ | | | | | 2 | $-\frac{\sqrt{21}xz(5x^4+10x^2y^2-20x^2z^2+5y^4-20y^2z^2+8z^4)}{8}$ |
| 46 | $\mathbb{Q}_{8,1}(E_{1g}, 1)$ | E_{1g} | 8 | Q, T | 1 | 1 | $\frac{3\sqrt{715}yz(7x^6-35x^4y^2+21x^2y^4-y^6)}{32}$ |
| 47 | $\mathbb{Q}_{8,2}(E_{1g}, 1)$ | | | | | 2 | $-\frac{3\sqrt{715}xz(x^6-21x^4y^2+35x^2y^4-7y^6)}{32}$ |
| 48 | $\mathbb{Q}_{1,1}(E_{1u})$ | E_{1u} | 1 | Q, T | - | 1 | x |

continued ...

Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|----|-------------------------------|----------|------|--------|--------------|-----------|--|
| 49 | $\mathbb{Q}_{1,2}(E_{1u})$ | | | | | 2 | y |
| 50 | $\mathbb{G}_{2,1}(E_{1u})$ | E_{1u} | 2 | G, M | - | 1 | $\sqrt{3}yz$ |
| 51 | $\mathbb{G}_{2,2}(E_{1u})$ | | | | | 2 | $-\sqrt{3}xz$ |
| 52 | $\mathbb{Q}_{3,1}(E_{1u})$ | E_{1u} | 3 | Q, T | - | 1 | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$ |
| 53 | $\mathbb{Q}_{3,2}(E_{1u})$ | | | | | 2 | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$ |
| 54 | $\mathbb{G}_{4,1}(E_{1u})$ | E_{1u} | 4 | G, M | - | 1 | $-\frac{\sqrt{10}yz(3x^2+3y^2-4z^2)}{4}$ |
| 55 | $\mathbb{G}_{4,2}(E_{1u})$ | | | | | 2 | $\frac{\sqrt{10}xz(3x^2+3y^2-4z^2)}{4}$ |
| 56 | $\mathbb{Q}_{5,1}(E_{1u}, 1)$ | E_{1u} | 5 | Q, T | 1 | 1 | $\frac{3\sqrt{14}x(x^4-10x^2y^2+5y^4)}{16}$ |
| 57 | $\mathbb{Q}_{5,2}(E_{1u}, 1)$ | | | | | 2 | $-\frac{3\sqrt{14}y(5x^4-10x^2y^2+y^4)}{16}$ |
| 58 | $\mathbb{Q}_{5,1}(E_{1u}, 2)$ | E_{1u} | 5 | Q, T | 2 | 1 | $\frac{\sqrt{15}x(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4)}{8}$ |
| 59 | $\mathbb{Q}_{5,2}(E_{1u}, 2)$ | | | | | 2 | $\frac{\sqrt{15}y(x^4+2x^2y^2-12x^2z^2+y^4-12y^2z^2+8z^4)}{8}$ |
| 60 | $\mathbb{Q}_{7,1}(E_{1u}, 1)$ | E_{1u} | 7 | Q, T | 1 | 1 | $\frac{\sqrt{429}x(x^6-21x^4y^2+35x^2y^4-7y^6)}{32}$ |
| 61 | $\mathbb{Q}_{7,2}(E_{1u}, 1)$ | | | | | 2 | $\frac{\sqrt{429}y(7x^6-35x^4y^2+21x^2y^4-y^6)}{32}$ |
| 62 | $\mathbb{Q}_{2,1}(E_{2g})$ | E_{2g} | 2 | Q, T | - | 1 | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| 63 | $\mathbb{Q}_{2,2}(E_{2g})$ | | | | | 2 | $-\sqrt{3}xy$ |
| 64 | $\mathbb{G}_{3,1}(E_{2g})$ | E_{2g} | 3 | G, M | - | 1 | $\sqrt{15}xyz$ |
| 65 | $\mathbb{G}_{3,2}(E_{2g})$ | | | | | 2 | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |
| 66 | $\mathbb{Q}_{4,1}(E_{2g}, 1)$ | E_{2g} | 4 | Q, T | 1 | 1 | $\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$ |
| 67 | $\mathbb{Q}_{4,2}(E_{2g}, 1)$ | | | | | 2 | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$ |
| 68 | $\mathbb{Q}_{4,1}(E_{2g}, 2)$ | E_{2g} | 4 | Q, T | 2 | 1 | $-\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$ |
| 69 | $\mathbb{Q}_{4,2}(E_{2g}, 2)$ | | | | | 2 | $\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$ |

continued ...

Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|----|-------------------------------|----------|------|--------|--------------|-----------|--|
| 70 | $\mathbb{Q}_{6,1}(E_{2g}, 1)$ | E_{2g} | 6 | Q, T | 1 | 1 | $-\frac{3\sqrt{7}(x^2+y^2-10z^2)(x^2-2xy-y^2)(x^2+2xy-y^2)}{16}$ |
| 71 | $\mathbb{Q}_{6,2}(E_{2g}, 1)$ | | | | | 2 | $-\frac{3\sqrt{7}xy(x-y)(x+y)(x^2+y^2-10z^2)}{4}$ |
| 72 | $\mathbb{Q}_{6,1}(E_{2g}, 2)$ | E_{2g} | 6 | Q, T | 2 | 1 | $\frac{\sqrt{210}(x-y)(x+y)(x^4+2x^2y^2-16x^2z^2+y^4-16y^2z^2+16z^4)}{32}$ |
| 73 | $\mathbb{Q}_{6,2}(E_{2g}, 2)$ | | | | | 2 | $-\frac{\sqrt{210}xy(x^4+2x^2y^2-16x^2z^2+y^4-16y^2z^2+16z^4)}{16}$ |
| 74 | $\mathbb{Q}_{8,1}(E_{2g}, 1)$ | E_{2g} | 8 | Q, T | 1 | 1 | $\frac{3\sqrt{715}(x^4-4x^3y-6x^2y^2+4xy^3+y^4)(x^4+4x^3y-6x^2y^2-4xy^3+y^4)}{128}$ |
| 75 | $\mathbb{Q}_{8,2}(E_{2g}, 1)$ | | | | | 2 | $-\frac{3\sqrt{715}xy(x-y)(x+y)(x^2-2xy-y^2)(x^2+2xy-y^2)}{16}$ |
| 76 | $\mathbb{G}_{2,1}(E_{2u})$ | E_{2u} | 2 | G, M | - | 1 | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| 77 | $\mathbb{G}_{2,2}(E_{2u})$ | | | | | 2 | $-\sqrt{3}xy$ |
| 78 | $\mathbb{Q}_{3,1}(E_{2u})$ | E_{2u} | 3 | Q, T | - | 1 | $\sqrt{15}xyz$ |
| 79 | $\mathbb{Q}_{3,2}(E_{2u})$ | | | | | 2 | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |
| 80 | $\mathbb{G}_{4,1}(E_{2u}, 1)$ | E_{2u} | 4 | G, M | 1 | 1 | $\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$ |
| 81 | $\mathbb{G}_{4,2}(E_{2u}, 1)$ | | | | | 2 | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$ |
| 82 | $\mathbb{G}_{4,1}(E_{2u}, 2)$ | E_{2u} | 4 | G, M | 2 | 1 | $-\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$ |
| 83 | $\mathbb{G}_{4,2}(E_{2u}, 2)$ | | | | | 2 | $\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$ |
| 84 | $\mathbb{Q}_{5,1}(E_{2u}, 1)$ | E_{2u} | 5 | Q, T | 1 | 1 | $-\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$ |
| 85 | $\mathbb{Q}_{5,2}(E_{2u}, 1)$ | | | | | 2 | $\frac{3\sqrt{35}z(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$ |
| 86 | $\mathbb{Q}_{5,1}(E_{2u}, 2)$ | E_{2u} | 5 | Q, T | 2 | 1 | $-\frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2}$ |
| 87 | $\mathbb{Q}_{5,2}(E_{2u}, 2)$ | | | | | 2 | $-\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$ |
| 88 | $\mathbb{Q}_{9,1}(E_{2u}, 1)$ | E_{2u} | 9 | Q, T | 1 | 1 | $\frac{3\sqrt{12155}xyz(x-y)(x+y)(x^2-2xy-y^2)(x^2+2xy-y^2)}{16}$ |
| 89 | $\mathbb{Q}_{9,2}(E_{2u}, 1)$ | | | | | 2 | $\frac{3\sqrt{12155}z(x^4-4x^3y-6x^2y^2+4xy^3+y^4)(x^4+4x^3y-6x^2y^2-4xy^3+y^4)}{128}$ |

— Basis in full matrix —

Table 3: dimension = 40

| # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) |
|----|-----------------------------|----|--------------------------------|----|--------------------------------|----|--------------------------------|----|-----------------------------|
| 0 | $ d_v\rangle @\text{Mn}(1)$ | 1 | $ d_{xy}\rangle @\text{Mn}(1)$ | 2 | $ d_{xz}\rangle @\text{Mn}(1)$ | 3 | $ d_{yz}\rangle @\text{Mn}(1)$ | 4 | $ d_u\rangle @\text{Mn}(1)$ |
| 5 | $ d_v\rangle @\text{Mn}(2)$ | 6 | $ d_{xy}\rangle @\text{Mn}(2)$ | 7 | $ d_{xz}\rangle @\text{Mn}(2)$ | 8 | $ d_{yz}\rangle @\text{Mn}(2)$ | 9 | $ d_u\rangle @\text{Mn}(2)$ |
| 10 | $ d_v\rangle @\text{Mn}(3)$ | 11 | $ d_{xy}\rangle @\text{Mn}(3)$ | 12 | $ d_{xz}\rangle @\text{Mn}(3)$ | 13 | $ d_{yz}\rangle @\text{Mn}(3)$ | 14 | $ d_u\rangle @\text{Mn}(3)$ |
| 15 | $ d_v\rangle @\text{Mn}(4)$ | 16 | $ d_{xy}\rangle @\text{Mn}(4)$ | 17 | $ d_{xz}\rangle @\text{Mn}(4)$ | 18 | $ d_{yz}\rangle @\text{Mn}(4)$ | 19 | $ d_u\rangle @\text{Mn}(4)$ |
| 20 | $ d_v\rangle @\text{Mn}(5)$ | 21 | $ d_{xy}\rangle @\text{Mn}(5)$ | 22 | $ d_{xz}\rangle @\text{Mn}(5)$ | 23 | $ d_{yz}\rangle @\text{Mn}(5)$ | 24 | $ d_u\rangle @\text{Mn}(5)$ |
| 25 | $ d_v\rangle @\text{Mn}(6)$ | 26 | $ d_{xy}\rangle @\text{Mn}(6)$ | 27 | $ d_{xz}\rangle @\text{Mn}(6)$ | 28 | $ d_{yz}\rangle @\text{Mn}(6)$ | 29 | $ d_u\rangle @\text{Mn}(6)$ |
| 30 | $ d_v\rangle @\text{Sn}(1)$ | 31 | $ d_{xy}\rangle @\text{Sn}(1)$ | 32 | $ d_{xz}\rangle @\text{Sn}(1)$ | 33 | $ d_{yz}\rangle @\text{Sn}(1)$ | 34 | $ d_u\rangle @\text{Sn}(1)$ |
| 35 | $ d_v\rangle @\text{Sn}(2)$ | 36 | $ d_{xy}\rangle @\text{Sn}(2)$ | 37 | $ d_{xz}\rangle @\text{Sn}(2)$ | 38 | $ d_{yz}\rangle @\text{Sn}(2)$ | 39 | $ d_u\rangle @\text{Sn}(2)$ |

Table 4: Atomic basis (orbital part only)

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

- Mn : 'Mn' site-cluster

* bra: $\langle d_v |, \langle d_{xy} |, \langle d_{xz} |, \langle d_{yz} |, \langle d_u |$

* ket: $|d_v \rangle, |d_{xy} \rangle, |d_{xz} \rangle, |d_{yz} \rangle, |d_u \rangle$

* wyckoff: 6h

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

$$\boxed{\text{z2}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

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

$$\boxed{\text{z4}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z5}} \quad \mathbb{Q}_4^{(c)}(A_{1g}) = \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z6}} \quad \mathbb{Q}_6^{(c)}(A_{1g}, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z41}} \quad \mathbb{Q}_7^{(c)}(A_{1u}) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_3^{(s)}(B_{1u})$$

$$\boxed{\text{z42}} \quad \mathbb{G}_2^{(c)}(A_{1u}) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z43}} \quad \mathbb{G}_4^{(c)}(A_{1u}) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z67}} \quad \mathbb{Q}_6^{(c)}(A_{2g}) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z68}} \quad \mathbb{G}_1^{(c)}(A_{2g}) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z69}} \quad \mathbb{G}_3^{(c)}(A_{2g}) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z95}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z96}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_3^{(s)}(B_{1u})$$

$$\boxed{\text{z97}} \quad \mathbb{Q}_3^{(c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z126}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z127}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, b) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z128}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z129}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{1u})$$

$$\boxed{\text{z130}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) = -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{1u})$$

$$\boxed{\text{z131}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, c) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z132}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, d) = \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{1u})$$

$$\boxed{\text{z133}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, e) = -\frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{58}$$

$$\boxed{\text{z134}} \quad \mathbb{Q}_5^{(c)}(B_{1u}) = -\frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{58} - \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{29}$$

$$\boxed{\text{z135}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z136}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, b) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z137}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z244}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z245}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) = \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{58}$$

$$\boxed{\text{z246}} \quad \mathbb{Q}_5^{(c)}(B_{2u}) = \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{29}$$

$$\boxed{\text{z247}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z248}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z249}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, b) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z250}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z251}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, c) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{8}$$

$$\boxed{\text{z252}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{8} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{8}$$

$$\boxed{\text{z253}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z254}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z255}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, b) = -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{8}$$

$$\boxed{\text{z256}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, b) = \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{8}$$

$$\boxed{\text{z257}} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 1) = -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z258}} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 1) = \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z259}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z260}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z261}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, b) = -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

$$\boxed{\text{z376}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

$$\boxed{\text{z377}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, c) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14}$$

$$\boxed{\text{z378}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, c) = -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14}$$

$$\boxed{\text{z404}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, d) = \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(s)}(B_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(s)}(B_{1u})}{58}$$

$$\boxed{\text{z405}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, d) = -\frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(s)}(B_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(s)}(B_{1u})}{58}$$

$$\boxed{\text{z406}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, a) = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{7}$$

$$\boxed{\text{z430}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, a) = -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{7}$$

$$\boxed{\text{z431}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, b) = \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(s)}(B_{1u})}{58} - \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(s)}(B_{1u})}{29}$$

$$\boxed{\text{z432}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, b) = -\frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(s)}(B_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(s)}(B_{1u})}{29}$$

$$\boxed{\text{z433}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, c) = \frac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14} - \frac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{7}$$

$$\boxed{\text{z434}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, c) = -\frac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14} - \frac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{7}$$

$$\boxed{\text{z435}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z465}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z466}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 2) = \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14} + \frac{\sqrt{70}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14}$$

$$\boxed{\text{z467}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 2) = -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{14} + \frac{\sqrt{70}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{14}$$

$$\boxed{\text{z491}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z492}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z493}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z494}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z495}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, c) = -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z496}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, c) = -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z497}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, d) = \frac{\sqrt{4970}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{142} - \frac{\sqrt{4970}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{142} + \frac{\sqrt{142}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{142}$$

$$\boxed{\text{z498}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, d) = -\frac{\sqrt{4970}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{142} - \frac{\sqrt{4970}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{142} + \frac{\sqrt{142}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{142}$$

$$\boxed{\text{z499}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1a) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z500}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1a) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z501}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1b) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z502}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1b) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z503}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1c) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z504}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1c) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{2}$$

$$\boxed{\text{z505}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2a) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z506}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2a) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z507}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2b) = \frac{\sqrt{71}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{142} - \frac{\sqrt{71}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{142} - \frac{\sqrt{2485}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{71}$$

$$\boxed{\text{z508}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2b) = -\frac{\sqrt{71}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{142} - \frac{\sqrt{71}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(s)}(E_{2g})}{142} - \frac{\sqrt{2485}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(s)}(E_{2g})}{71}$$

$$\boxed{\text{z613}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

$$\boxed{\text{z614}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

$$\boxed{\text{z615}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z616}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, b) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z617}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, c) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

$$\boxed{\text{z618}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

$$\boxed{\text{z619}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, d) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{8}$$

$$\boxed{\text{z620}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, d) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{8}$$

$$\boxed{\text{z621}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1) = -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z622}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1) = \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{2}$$

$$\boxed{\text{z623}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 2) = \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{8} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{8}$$

$$\boxed{\text{z624}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 2) = -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(s)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(s)}(E_{1u})}{8}$$

• Sn : 'Sn' site-cluster

* bra: $\langle d_v |, \langle d_{xy} |, \langle d_{xz} |, \langle d_{yz} |, \langle d_u |$

* ket: $|d_v\rangle, |d_{xy}\rangle, |d_{xz}\rangle, |d_{yz}\rangle, |d_u\rangle$

* wyckoff: 2c

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

$$\boxed{\text{z8}} \quad \mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z9}} \quad \mathbb{Q}_4^{(c)}(A_{1g}) = \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z70}} \quad \mathbb{Q}_7^{(c)}(A_{1u}) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_3^{(s)}(B_{1u})$$

$$\boxed{\text{z98}} \quad \mathbb{Q}_1^{(c)}(A_{2u}) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_3^{(s)}(B_{1u})$$

$$\boxed{\text{z138}} \quad \mathbb{Q}_4^{(c)}(B_{1g}) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z139}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{1u})$$

$$\boxed{\text{z140}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) = -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{1u})$$

$$\boxed{\text{z141}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, c) = \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{1u})$$

$$\boxed{\text{z262}} \quad \mathbb{Q}_4^{(c)}(B_{2g}) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z263}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z264}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z265}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z266}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z267}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

$$\boxed{\text{z379}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

$$\boxed{\text{z407}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, b) = \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(s)}(B_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(s)}(B_{1u})}{58}$$

$$\boxed{\text{z436}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, b) = -\frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(s)}(B_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(s)}(B_{1u})}{58}$$

$$\boxed{\text{z437}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}) = \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(s)}(B_{1u})}{58} - \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(s)}(B_{1u})}{29}$$

$$\boxed{\text{z438}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}) = -\frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(s)}(B_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(s)}(B_{1u})}{29}$$

$$\boxed{\text{z509}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z510}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z511}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z512}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z513}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z514}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z625}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

$$\boxed{\text{z626}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

$$\boxed{\text{z627}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, b) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

$$\boxed{\text{z628}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, b) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(s)}(B_{1u})}{2}$$

- Mn;Mn_001_1 : 'Mn'-'Mn' bond-cluster

* bra: $\langle d_v |$, $\langle d_{xy} |$, $\langle d_{xz} |$, $\langle d_{yz} |$, $\langle d_u |$

* ket: $|d_v \rangle$, $|d_{xy} \rangle$, $|d_{xz} \rangle$, $|d_{yz} \rangle$, $|d_u \rangle$

* wyckoff: 6b6h

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

$$\boxed{\text{z11}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z12}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, c) = \mathbb{M}_1^{(a)}(A_{2g})\mathbb{M}_1^{(b)}(A_{2g})$$

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

$$\boxed{\text{z14}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z15}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, c) = \mathbb{M}_3^{(a)}(A_{2g})\mathbb{M}_1^{(b)}(A_{2g})$$

$$\boxed{\text{z16}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, d) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z17}} \quad \mathbb{Q}_4^{(c)}(A_{1g}) = \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z18}} \quad \mathbb{Q}_6^{(c)}(A_{1g}, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z44}} \quad \mathbb{Q}_7^{(c)}(A_{1u}) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z45}} \quad \mathbb{G}_0^{(c)}(A_{1u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z46}} \quad \mathbb{G}_0^{(c)}(A_{1u}, b) = \mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z47}} \quad \mathbb{G}_2^{(c)}(A_{1u}, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z71}} \quad \mathbb{G}_2^{(c)}(A_{1u}, b) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z72}} \quad \mathbb{G}_4^{(c)}(A_{1u}) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z73}} \quad \mathbb{Q}_6^{(c)}(A_{2g}) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z74}} \quad \mathbb{G}_1^{(c)}(A_{2g}, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z75}} \quad \mathbb{G}_1^{(c)}(A_{2g}, b) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z76}} \quad \mathbb{G}_3^{(c)}(A_{2g}) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z99}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z100}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z101}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, c) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z102}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, d) = -\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z103}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, a) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z104}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, b) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z142}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z143}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, b) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z144}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z145}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, d) = \mathbb{M}_3^{(a)}(B_{2g})\mathbb{M}_1^{(b)}(A_{2g})$$

$$\boxed{\text{z146}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, e) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z147}} \quad \mathbb{G}_3^{(c)}(B_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z148}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z149}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) = -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z150}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, c) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z151}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, d) = \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z152}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, e) = -\frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{58}$$

$$\boxed{\text{z153}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, f) = \mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z154}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, g) = -\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z155}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, h) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z156}} \quad \mathbb{Q}_5^{(c)}(B_{1u}) = -\frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{58} - \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{29}$$

$$\boxed{\text{z157}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z158}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, b) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z159}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z160}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, d) = \mathbb{M}_3^{(a)}(B_{1g})\mathbb{M}_1^{(b)}(A_{2g})$$

$$\boxed{\text{z161}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, e) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z162}} \quad \mathbb{G}_3^{(c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z163}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z164}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) = \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{58}$$

$$\boxed{\text{z165}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, c) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z268}} \quad \mathbb{Q}_5^{(c)}(B_{2u}) = \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{29}$$

$$\boxed{\text{z269}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

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

$$\boxed{\text{z271}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, b) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z272}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z273}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, c) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8}$$

$$\boxed{\text{z274}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8}$$

$$\boxed{\text{z275}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, d) = \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{M}_1^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z276}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, d) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{M}_1^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z277}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, e) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z278}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, e) = \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z279}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, f) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{M}_1^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z280}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, f) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{M}_1^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z281}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, g) = \frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{8}$$

$$\boxed{\text{z282}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, g) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{8}$$

$$\boxed{\text{z283}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z284}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z285}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, b) = -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8}$$

$$\boxed{\text{z286}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, b) = \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8}$$

$$\boxed{\text{z287}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, c) = -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{8}$$

$$\boxed{\text{z288}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, c) = \frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{8}$$

$$\boxed{\text{z289}} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 1) = -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z290}} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 1) = \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z291}} \quad \mathbb{G}_{5,1}^{(c)}(E_{1g}, 1) = \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z292}} \quad \mathbb{G}_{5,2}^{(c)}(E_{1g}, 1) = -\frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z293}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z380}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z381}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, b) = -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z382}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z383}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, c) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14}$$

$$\boxed{\text{z384}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, c) = -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14}$$

$$\boxed{\text{z385}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, d) = \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{58}$$

$$\boxed{\text{z408}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, d) = -\frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{58}$$

$$\boxed{\text{z409}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, e) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z410}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, e) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z411}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, f) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z412}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, f) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z413}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, a) = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{7}$$

$$\boxed{\text{z439}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, a) = -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{7}$$

$$\boxed{\text{z440}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, b) = \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{58} - \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{29}$$

$$\boxed{\text{z441}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, b) = -\frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{29}$$

$$\boxed{\text{z442}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, c) = \frac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{7}$$

$$\boxed{\text{z443}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, c) = -\frac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{7}$$

$$\boxed{\text{z444}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, d) = -\frac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{22} + \frac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{22} - \frac{\sqrt{33}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{11}$$

$$\boxed{\text{z445}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, d) = \frac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{22} + \frac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{22} + \frac{\sqrt{33}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{11}$$

$$\boxed{\text{z446}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z447}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z448}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 2) = \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} + \frac{\sqrt{70}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14}$$

$$\boxed{\text{z469}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 2) = -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} + \frac{\sqrt{70}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14}$$

$$\boxed{\text{z470}} \quad \mathbb{G}_{2,1}^{(c)}(E_{1u}) = \frac{\sqrt{66}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{22} - \frac{\sqrt{66}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{22} - \frac{\sqrt{110}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{22}$$

$$\boxed{\text{z471}} \quad \mathbb{G}_{2,2}^{(c)}(E_{1u}) = -\frac{\sqrt{66}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{22} - \frac{\sqrt{66}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{22} + \frac{\sqrt{110}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{22}$$

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

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

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

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

$$\boxed{\text{z519}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, c) = -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z520}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, c) = -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z521}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, d) = \frac{\sqrt{4970}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142} - \frac{\sqrt{4970}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142} + \frac{\sqrt{142}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142}$$

$$\boxed{\text{z522}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, d) = -\frac{\sqrt{4970}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142} - \frac{\sqrt{4970}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142} + \frac{\sqrt{142}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142}$$

$$\boxed{\text{z523}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, e) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z524}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, e) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z525}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, f) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{M}_1^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z526}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, f) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{M}_1^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z527}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, g) = -\frac{\sqrt{2}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z528}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, g) = \frac{\sqrt{2}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z529}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1a) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z530}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1a) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z531}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1b) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z532}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1b) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z533}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1c) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z534}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1c) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z535}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1d) = -\frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z536}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1d) = \frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z537}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2a) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z538}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2a) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z539}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2b) = \frac{\sqrt{71}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142} - \frac{\sqrt{71}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142} - \frac{\sqrt{2485}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{71}$$

$$\boxed{\text{z540}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2b) = -\frac{\sqrt{71}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142} - \frac{\sqrt{71}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142} - \frac{\sqrt{2485}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{71}$$

$$\boxed{\text{z629}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z630}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z631}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z632}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, b) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z633}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, c) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z634}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z635}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, d) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8}$$

$$\boxed{\text{z636}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, d) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8}$$

$$\boxed{\text{z637}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, e) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z638}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, e) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z639}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, f) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z640}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, f) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z641}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, g) = \frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{8}$$

$$\boxed{\text{z642}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, g) = -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{8}$$

$$\boxed{\text{z643}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1) = -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z644}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1) = \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z645}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 2) = \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8}$$

$$\boxed{\text{z646}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 2) = -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8}$$

$$\boxed{\text{z647}} \quad \mathbb{G}_{2,1}^{(c)}(E_{2u}, a) = \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z648}} \quad \mathbb{G}_{2,2}^{(c)}(E_{2u}, a) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z649}} \quad \mathbb{G}_{2,1}^{(c)}(E_{2u}, b) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{8}$$

$$\boxed{\text{z650}} \quad \mathbb{G}_{2,2}^{(c)}(E_{2u}, b) = \frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{8}$$

$$\boxed{\text{z651}} \quad \mathbb{G}_{4,1}^{(c)}(E_{2u}, 1) = -\frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z652}} \quad \mathbb{G}_{4,2}^{(c)}(E_{2u}, 1) = \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2}$$

• Sn; Mn_001_1 : 'Mn'-'Sn' bond-cluster

- * bra: $\langle d_v |, \langle d_{xy} |, \langle d_{xz} |, \langle d_{yz} |, \langle d_u |$
- * ket: $|d_v \rangle, |d_{xy} \rangle, |d_{xz} \rangle, |d_{yz} \rangle, |d_u \rangle$
- * wyckoff: 12a@12j

$$\boxed{\text{z19}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z20}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z21}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, c) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z22}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, d) = \mathbb{M}_1^{(a)}(A_{2g})\mathbb{M}_1^{(b)}(A_{2g})$$

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

$$\boxed{\text{z24}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z25}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, c) = \mathbb{M}_3^{(a)}(A_{2g})\mathbb{M}_1^{(b)}(A_{2g})$$

$$\boxed{\text{z26}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, d) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z27}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, e) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z28}} \quad \mathbb{Q}_4^{(c)}(A_{1g}) = \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z29}} \quad \mathbb{Q}_6^{(c)}(A_{1g}, 2a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z30}} \quad \mathbb{Q}_6^{(c)}(A_{1g}, 2b) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z31}} \quad \mathbb{Q}_6^{(c)}(A_{1g}, 2c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z48}} \quad \mathbb{Q}_7^{(c)}(A_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z49}} \quad \mathbb{Q}_7^{(c)}(A_{1u}, b) = \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z50}} \quad \mathbb{Q}_7^{(c)}(A_{1u}, c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z51}} \quad \mathbb{G}_0^{(c)}(A_{1u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z52}} \quad \mathbb{G}_0^{(c)}(A_{1u}, b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2}$$

$$\boxed{\text{z53}} \quad \mathbb{G}_0^{(c)}(A_{1u}, c) = \frac{\sqrt{2}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2} + \frac{\sqrt{2}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z54}} \quad \mathbb{G}_2^{(c)}(A_{1u}, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z55}} \quad \mathbb{G}_2^{(c)}(A_{1u}, b) = \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z56}} \quad \mathbb{G}_2^{(c)}(A_{1u}, c) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z57}} \quad \mathbb{G}_2^{(c)}(A_{1u}, d) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2}$$

$$\boxed{\text{z58}} \quad \mathbb{G}_4^{(c)}(A_{1u}) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z59}} \quad \mathbb{G}_6^{(c)}(A_{1u}, 2) = -\frac{\sqrt{2}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2} + \frac{\sqrt{2}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z60}} \quad \mathbb{Q}_6^{(c)}(A_{2g}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_6^{(b)}(A_{2g})$$

$$\boxed{\text{z77}} \quad \mathbb{Q}_6^{(c)}(A_{2g}, b) = -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_6^{(b)}(A_{2g})$$

$$\boxed{\text{z78}} \quad \mathbb{Q}_6^{(c)}(A_{2g}, c) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z79}} \quad \mathbb{Q}_6^{(c)}(A_{2g}, d) = \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_6^{(b)}(A_{2g})$$

$$\boxed{\text{z80}} \quad \mathbb{Q}_6^{(c)}(A_{2g}, e) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z81}} \quad \mathbb{Q}_6^{(c)}(A_{2g}, f) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z82}} \quad \mathbb{G}_1^{(c)}(A_{2g}, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z83}} \quad \mathbb{G}_1^{(c)}(A_{2g}, b) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z84}} \quad \mathbb{G}_1^{(c)}(A_{2g}, c) = \mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z85}} \quad \mathbb{G}_1^{(c)}(A_{2g}, d) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z86}} \quad \mathbb{G}_1^{(c)}(A_{2g}, e) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z87}} \quad \mathbb{G}_3^{(c)}(A_{2g}, a) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z88}} \quad \mathbb{G}_3^{(c)}(A_{2g}, b) = \mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z105}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z106}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z107}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, c) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z108}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, d) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2}$$

$$\boxed{\text{z109}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, e) = -\frac{\sqrt{2}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z110}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, a) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z111}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, b) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z112}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, c) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2}$$

$$\boxed{\text{z113}} \quad \mathbb{Q}_7^{(c)}(A_{2u}, 2a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z114}} \quad \mathbb{Q}_7^{(c)}(A_{2u}, 2b) = \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z115}} \quad \mathbb{Q}_7^{(c)}(A_{2u}, 2c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z116}} \quad \mathbb{G}_6^{(c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z166}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z167}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z168}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, c) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z169}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, d) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_6^{(b)}(A_{2g})$$

$$\boxed{\text{z170}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, e) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z171}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, f) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z172}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, g) = \mathbb{M}_3^{(a)}(B_{2g})\mathbb{M}_1^{(b)}(A_{2g})$$

$$\boxed{\text{z173}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, h) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z174}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, i) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z175}} \quad \mathbb{G}_3^{(c)}(B_{1g}, a) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z176}} \quad \mathbb{G}_3^{(c)}(B_{1g}, b) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z177}} \quad \mathbb{G}_3^{(c)}(B_{1g}, c) = \mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z178}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z179}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) = -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z180}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, c) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z181}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, d) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z182}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, e) = \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z183}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, f) = -\frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{58}$$

$$\boxed{\text{z184}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, g) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z185}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, h) = \mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z186}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, i) = -\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z187}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, j) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z188}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, k) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2}$$

$$\boxed{\text{z189}} \quad \mathbb{Q}_5^{(c)}(B_{1u}) = -\frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{58} - \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{29}$$

$$\boxed{\text{z190}} \quad \mathbb{Q}_9^{(c)}(B_{1u}, 1) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z191}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z192}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, b) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z193}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, c) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z194}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, d) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_6^{(b)}(A_{2g})$$

$$\boxed{\text{z195}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, e) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z196}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, f) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z197}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, g) = \mathbb{M}_3^{(a)}(B_{1g})\mathbb{M}_1^{(b)}(A_{2g})$$

$$\boxed{\text{z198}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, h) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z199}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, i) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z200}} \quad \mathbb{G}_3^{(c)}(B_{2g}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z201}} \quad \mathbb{G}_3^{(c)}(B_{2g}, b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z202}} \quad \mathbb{G}_3^{(c)}(B_{2g}, c) = \mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z203}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z204}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) = -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z205}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, c) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z206}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, d) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z207}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, e) = \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z208}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, f) = \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{29} - \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{58}$$

$$\boxed{\text{z209}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, g) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

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

$$\boxed{\text{z211}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, i) = \mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z212}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, j) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z213}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, k) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2}$$

$$\boxed{\text{z294}} \quad \mathbb{Q}_5^{(c)}(B_{2u}) = \frac{\sqrt{58}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{29} + \frac{\sqrt{58}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{58} + \frac{\sqrt{406}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{29}$$

$$\boxed{\text{z295}} \quad \mathbb{Q}_9^{(c)}(B_{2u}, 1) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z296}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

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

$$\boxed{\text{z298}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, b) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z299}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z300}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, c) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8}$$

$$\boxed{\text{z301}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8}$$

$$\boxed{\text{z302}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, d) = \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z303}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, d) = -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z304}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, e) = \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{M}_1^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z305}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, e) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{M}_1^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z306}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, f) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z307}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, f) = \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z308}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, g) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z309}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, g) = \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z310}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, h) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{M}_1^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z311}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, h) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{M}_1^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z312}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, i) = \frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{8}$$

$$\boxed{\text{z313}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, i) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{8}$$

$$\boxed{\text{z314}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, j) = \frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{8}$$

$$\boxed{\text{z315}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, j) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{8}$$

$$\boxed{\text{z316}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z317}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z318}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, b) = -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8}$$

$$\boxed{\text{z319}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, b) = \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8} + \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{8}$$

$$\boxed{\text{z320}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, c) = -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{8} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{8}$$

$$\boxed{\text{z321}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, c) = \frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{8} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{8}$$

$$\boxed{\text{z322}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, d) = -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{8} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{8}$$

$$\boxed{\text{z323}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, d) = \frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{8} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{8}$$

$$\boxed{\text{z324}} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 1a) = -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_6^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z325}} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 1a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_6^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z326}} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 1b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z327}} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 1b) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z328}} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 1c) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_6^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z329}} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 1c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_6^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z330}} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 1d) = -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z331}} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 1d) = \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z332}} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 1e) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z333}} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 1e) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z334}} \quad \mathbb{Q}_{8,1}^{(c)}(E_{1g}, 1) = \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z335}} \quad \mathbb{Q}_{8,2}^{(c)}(E_{1g}, 1) = -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z336}} \quad \mathbb{G}_{1,1}^{(c)}(E_{1g}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z337}} \quad \mathbb{G}_{1,2}^{(c)}(E_{1g}) = \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z338}} \quad \mathbb{G}_{3,1}^{(c)}(E_{1g}) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z339}} \quad \mathbb{G}_{3,2}^{(c)}(E_{1g}) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z340}} \quad \mathbb{G}_{5,1}^{(c)}(E_{1g}, 1a) = \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z341}} \quad \mathbb{G}_{5,2}^{(c)}(E_{1g}, 1a) = -\frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z342}} \quad \mathbb{G}_{5,1}^{(c)}(E_{1g}, 1b) = \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z343}} \quad \mathbb{G}_{5,2}^{(c)}(E_{1g}, 1b) = -\frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z344}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z345}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z386}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z387}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z388}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, c) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14}$$

$$\boxed{\text{z389}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, c) = -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14}$$

$$\boxed{\text{z390}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, d) = \frac{\sqrt{203}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{29} - \frac{\sqrt{29}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{58} + \frac{\sqrt{203}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{29} + \frac{\sqrt{29}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{58}$$

$$\boxed{\text{z391}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, d) = -\frac{\sqrt{203}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{29} - \frac{\sqrt{29}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{58} + \frac{\sqrt{203}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{29} - \frac{\sqrt{29}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{58}$$

$$\boxed{\text{z392}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, e) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z393}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, e) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z394}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, f) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z395}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, f) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z396}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, g) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2}$$

$$\boxed{\text{z397}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, g) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2}$$

$$\boxed{\text{z414}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, h) = \frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z415}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, h) = \frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{1u})}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z416}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, a) = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{7}$$

$$\boxed{\text{z417}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, a) = -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{7}$$

$$\boxed{\text{z418}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, b) = \frac{\sqrt{29}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{58} + \frac{\sqrt{203}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{29} + \frac{\sqrt{29}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{58} - \frac{\sqrt{203}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{29}$$

$$\boxed{\text{z419}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, b) = -\frac{\sqrt{29}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{58} + \frac{\sqrt{203}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{29} + \frac{\sqrt{29}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{58} + \frac{\sqrt{203}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{29}$$

$$\boxed{\text{z420}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, c) = \frac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{7}$$

$$\boxed{\text{z421}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, c) = -\frac{\sqrt{35}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{35}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{7}$$

$$\boxed{\text{z422}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, d) = -\frac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{22} + \frac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{22} - \frac{\sqrt{33}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{11}$$

$$\boxed{\text{z423}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, d) = \frac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{22} + \frac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{22} + \frac{\sqrt{33}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{11}$$

$$\boxed{\text{z424}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, e) = -\frac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{22} + \frac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{22} - \frac{\sqrt{33}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{11}$$

$$\boxed{\text{z425}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, e) = \frac{\sqrt{55}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{22} + \frac{\sqrt{55}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{22} + \frac{\sqrt{33}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{11}$$

$$\boxed{\text{z448}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z449}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z450}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z451}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1b) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z452}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1c) = -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z453}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1c) = -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z454}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1d) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z455}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1d) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{1u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z456}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1e) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z457}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1e) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z458}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1f) = \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z459}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1f) = \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z460}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1g) = -\frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z472}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1g) = \frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{1u})}{2} - \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z473}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 2) = \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} + \frac{\sqrt{70}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14}$$

$$\boxed{\text{z474}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 2) = -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{14} + \frac{\sqrt{70}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{14}$$

$$\boxed{\text{z475}} \quad \mathbb{Q}_{7,1}^{(c)}(E_{1u}, 1a) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z476}} \quad \mathbb{Q}_{7,2}^{(c)}(E_{1u}, 1a) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z477}} \quad \mathbb{Q}_{7,1}^{(c)}(E_{1u}, 1b) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z478}} \quad \mathbb{Q}_{7,2}^{(c)}(E_{1u}, 1b) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{1u})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z479}} \quad \mathbb{Q}_{7,1}^{(c)}(E_{1u}, 1c) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z480}} \quad \mathbb{Q}_{7,2}^{(c)}(E_{1u}, 1c) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z481}} \quad \mathbb{G}_{2,1}^{(c)}(E_{1u}, a) = \frac{\sqrt{66}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{22} - \frac{\sqrt{66}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{22} - \frac{\sqrt{110}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{22}$$

$$\boxed{\text{z482}} \quad \mathbb{G}_{2,2}^{(c)}(E_{1u}, a) = -\frac{\sqrt{66}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{22} - \frac{\sqrt{66}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{22} + \frac{\sqrt{110}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{22}$$

$$\boxed{\text{z483}} \quad \mathbb{G}_{2,1}^{(c)}(E_{1u}, b) = \frac{\sqrt{66}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{22} - \frac{\sqrt{66}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{22} - \frac{\sqrt{110}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{22}$$

$$\boxed{\text{z484}} \quad \mathbb{G}_{2,2}^{(c)}(E_{1u}, b) = -\frac{\sqrt{66}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{22} - \frac{\sqrt{66}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{22} + \frac{\sqrt{110}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{22}$$

$$\boxed{\text{z541}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z542}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z543}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z544}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z545}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, c) = -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z546}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, c) = -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z547}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, d) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z548}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, d) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z549}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, e) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_6^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z550}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, e) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_6^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z551}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, f) = \frac{\sqrt{4970}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142} - \frac{\sqrt{4970}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142} + \frac{\sqrt{142}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142}$$

$$\boxed{\text{z552}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, f) = -\frac{\sqrt{4970}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142} - \frac{\sqrt{4970}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142} + \frac{\sqrt{142}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142}$$

$$\boxed{\text{z553}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, g) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z554}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, g) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z555}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, h) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z556}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, h) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z557}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, i) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z558}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, i) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z559}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, j) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{M}_1^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z560}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, j) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{M}_1^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z561}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, k) = -\frac{\sqrt{2}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z562}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, k) = \frac{\sqrt{2}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z563}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, l) = -\frac{\sqrt{2}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z564}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, l) = \frac{\sqrt{2}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z565}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z566}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z567}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1b) = -\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_6^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z568}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_6^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z569}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1c) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z570}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1c) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z571}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1d) = -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z572}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1d) = -\frac{\sqrt{2}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z573}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1e) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z574}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1e) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z575}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1f) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_6^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z576}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1f) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_6^{(b)}(A_{2g})}{2}$$

$$\boxed{\text{z577}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1g) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z578}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1g) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z579}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1h) = \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z580}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1h) = \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z581}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1i) = -\frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z582}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1i) = \frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, a)}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, a)}{2}$$

$$\boxed{\text{z583}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1j) = -\frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z584}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1j) = \frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{2,2}^{(b)}(E_{2g}, b)}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{2,1}^{(b)}(E_{2g}, b)}{2}$$

$$\boxed{\text{z585}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2a) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z586}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2a) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z587}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2b) = \frac{\sqrt{71}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142} - \frac{\sqrt{71}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142} - \frac{\sqrt{2485}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{71}$$

$$\boxed{\text{z588}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2b) = -\frac{\sqrt{71}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{142} - \frac{\sqrt{71}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{142} - \frac{\sqrt{2485}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{71}$$

$$\boxed{\text{z589}} \quad \mathbb{Q}_{8,1}^{(c)}(E_{2g}, 1) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z590}} \quad \mathbb{Q}_{8,2}^{(c)}(E_{2g}, 1) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{4,2}^{(b)}(E_{2g}, 1)}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{4,1}^{(b)}(E_{2g}, 1)}{2}$$

$$\boxed{\text{z591}} \quad \mathbb{G}_{3,1}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z592}} \quad \mathbb{G}_{3,2}^{(c)}(E_{2g}) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z653}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, a) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z654}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, a) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z655}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z656}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, b) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z657}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, c) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z658}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, c) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z659}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, d) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8}$$

$$\boxed{\text{z660}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, d) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8}$$

$$\boxed{\text{z661}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, e) = -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z662}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, e) = \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z663}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, f) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z664}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, f) = \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z665}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, g) = \frac{\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z666}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, g) = -\frac{\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z667}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, h) = \frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{8}$$

$$\boxed{\text{z668}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, h) = -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{8}$$

$$\boxed{\text{z669}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, i) = \frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{8}$$

$$\boxed{\text{z670}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, i) = -\frac{\sqrt{10}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{8}$$

$$\boxed{\text{z671}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1a) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z672}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1a) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z673}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z674}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1b) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z675}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1c) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z676}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1c) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{1u})}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z677}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1d) = -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z678}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1d) = \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z679}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1e) = -\frac{\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z680}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1e) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z681}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1f) = -\frac{\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z682}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1f) = -\frac{\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2} - \frac{\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z683}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 2) = \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8}$$

$$\boxed{\text{z684}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 2) = -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8} - \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{1,1}^{(b)}(E_{1u})}{8} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{1,2}^{(b)}(E_{1u})}{8}$$

$$\boxed{\text{z685}} \quad \mathbb{Q}_{9,1}^{(c)}(E_{2u}, 1) = -\frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z686}} \quad \mathbb{Q}_{9,2}^{(c)}(E_{2u}, 1) = \frac{\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{5,1}^{(b)}(E_{1u}, 1)}{2} + \frac{\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{5,2}^{(b)}(E_{1u}, 1)}{2}$$

$$\boxed{\text{z687}} \quad \mathbb{G}_{2,1}^{(c)}(E_{2u}, a) = \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z688}} \quad \mathbb{G}_{2,2}^{(c)}(E_{2u}, a) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z689}} \quad \mathbb{G}_{2,1}^{(c)}(E_{2u}, b) = \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2}$$

$$\boxed{\text{z690}} \quad \mathbb{G}_{2,2}^{(c)}(E_{2u}, b) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2}$$

$$\boxed{\text{z691}} \quad \mathbb{G}_{2,1}^{(c)}(E_{2u}, c) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{8}$$

$$\boxed{\text{z692}} \quad \mathbb{G}_{2,2}^{(c)}(E_{2u}, c) = \frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{8}$$

$$\boxed{\text{z693}} \quad \mathbb{G}_{2,1}^{(c)}(E_{2u}, d) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{8}$$

$$\boxed{\text{z694}} \quad \mathbb{G}_{2,2}^{(c)}(E_{2u}, d) = \frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{8}$$

$$\boxed{\text{z695}} \quad \mathbb{G}_{4,1}^{(c)}(E_{2u}, 1a) = \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z696}} \quad \mathbb{G}_{4,2}^{(c)}(E_{2u}, 1a) = \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z697}} \quad \mathbb{G}_{4,1}^{(c)}(E_{2u}, 1b) = -\frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z698}} \quad \mathbb{G}_{4,2}^{(c)}(E_{2u}, 1b) = \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, a)}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, a)}{2}$$

$$\boxed{\text{z699}} \quad \mathbb{G}_{4,1}^{(c)}(E_{2u}, 1c) = -\frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2}$$

$$\boxed{\text{z700}} \quad \mathbb{G}_{4,2}^{(c)}(E_{2u}, 1c) = \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u}, b)}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u}, b)}{2}$$

• Sn;Sn_001_1 : 'Sn'-'Sn' bond-cluster

* bra: $\langle d_v |, \langle d_{xy} |, \langle d_{xz} |, \langle d_{yz} |, \langle d_u |$

* ket: $|d_v\rangle, |d_{xy}\rangle, |d_{xz}\rangle, |d_{yz}\rangle, |d_u\rangle$

* wyckoff: 6a@6g

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

$$\boxed{\text{z33}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{2} + \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z34}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, c) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_4^{(b)}(B_{2g})$$

$$\boxed{\text{z35}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, a) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z36}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{2} - \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z37}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, c) = \frac{\sqrt{3}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{3} + \frac{\sqrt{6}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6} + \frac{\sqrt{3}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{3} + \frac{\sqrt{6}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6}$$

$$\boxed{\text{z38}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, a) = \mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z39}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, b) = \frac{\sqrt{6}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} - \frac{\sqrt{3}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{3} + \frac{\sqrt{6}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{3}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{3}$$

$$\boxed{\text{z40}} \quad \mathbb{Q}_6^{(c)}(A_{1g}, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z61}} \quad \mathbb{G}_0^{(c)}(A_{1u}, a) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z62}} \quad \mathbb{G}_0^{(c)}(A_{1u}, b) = \mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z63}} \quad \mathbb{G}_2^{(c)}(A_{1u}, a) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z64}} \quad \mathbb{G}_2^{(c)}(A_{1u}, b) = \frac{\sqrt{14}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{7} + \frac{\sqrt{14}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{7} + \frac{\sqrt{21}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z65}} \quad \mathbb{G}_2^{(c)}(A_{1u}, c) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2}$$

$$\boxed{\text{z66}} \quad \mathbb{G}_4^{(c)}(A_{1u}) = -\frac{\sqrt{42}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{14} - \frac{\sqrt{42}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{14} + \frac{2\sqrt{7}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z89}} \quad \mathbb{Q}_6^{(c)}(A_{2g}, a) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_4^{(b)}(B_{2g})$$

$$\boxed{\text{z90}} \quad \mathbb{Q}_6^{(c)}(A_{2g}, b) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z91}} \quad \mathbb{G}_1^{(c)}(A_{2g}) = \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{10} - \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{5} - \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{5}$$

$$\boxed{\text{z92}} \quad \mathbb{G}_3^{(c)}(A_{2g}, a) = \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{5} + \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{10} - \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{5} - \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{10}$$

$$\boxed{\text{z93}} \quad \mathbb{G}_3^{(c)}(A_{2g}, b) = \frac{\sqrt{6}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{3}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{3} - \frac{\sqrt{6}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} + \frac{\sqrt{3}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{3}$$

$$\boxed{\text{z94}} \quad \mathbb{G}_5^{(c)}(A_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{3} + \frac{\sqrt{6}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6} - \frac{\sqrt{3}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{3} - \frac{\sqrt{6}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6}$$

$$\boxed{\text{z117}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z118}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z119}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, c) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2}$$

$$\boxed{\text{z120}} \quad \mathbb{Q}_3^{(c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z121}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, a) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{2}$$

$$\boxed{\text{z122}} \quad \mathbb{Q}_4^{(c)}(B_{1g}, b) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z123}} \quad \begin{aligned} \mathbb{Q}_4^{(c)}(B_{1g}, c) = & -\frac{3\sqrt{71}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{71} - \frac{\sqrt{994}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{71} - \frac{5\sqrt{142}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{142} \\ & + \frac{3\sqrt{71}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{71} + \frac{\sqrt{994}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{71} + \frac{5\sqrt{142}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{142} \end{aligned}$$

$$\boxed{\text{z124}} \quad \begin{aligned} \mathbb{Q}_6^{(c)}(B_{1g}) = & \frac{7\sqrt{497}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{355} + \frac{9\sqrt{142}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{710} - \frac{6\sqrt{994}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{355} \\ & - \frac{7\sqrt{497}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{355} - \frac{9\sqrt{142}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{710} + \frac{6\sqrt{994}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{355} \end{aligned}$$

$$\boxed{\text{z125}} \quad \mathbb{G}_3^{(c)}(B_{1g}, a) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{2}$$

$$\boxed{\text{z214}} \quad \mathbb{G}_3^{(c)}(B_{1g}, b) = -\frac{3\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{10} + \frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{5} - \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{5} + \frac{3\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{10} - \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{5} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{5}$$

$$\boxed{\text{z215}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2}$$

$$\boxed{\text{z216}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{4} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{4} - \frac{\sqrt{3}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z217}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, c) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2}$$

$$\boxed{\text{z218}} \quad \mathbb{G}_4^{(c)}(B_{1u}) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{4} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{4} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z219}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_4^{(b)}(B_{2g})$$

$$\boxed{\text{z220}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, b) = -\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_4^{(b)}(B_{2g})$$

$$\boxed{\text{z221}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, c) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{2}$$

$$\boxed{\text{z222}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, d) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z223}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, e) = -\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_4^{(b)}(B_{2g})$$

$$\begin{aligned} \boxed{\text{z224}} \quad \mathbb{Q}_4^{(c)}(B_{2g}, f) = & -\frac{3\sqrt{71}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{71} - \frac{\sqrt{994}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{71} + \frac{5\sqrt{142}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{142} \\ & - \frac{3\sqrt{71}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{71} - \frac{\sqrt{994}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{71} + \frac{5\sqrt{142}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{142} \end{aligned}$$

$$\begin{aligned} \boxed{\text{z225}} \quad \mathbb{Q}_6^{(c)}(B_{2g}) = & \frac{7\sqrt{497}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{355} + \frac{9\sqrt{142}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{710} + \frac{6\sqrt{994}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{355} \\ & + \frac{7\sqrt{497}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{355} + \frac{9\sqrt{142}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{710} + \frac{6\sqrt{994}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{355} \end{aligned}$$

$$\boxed{\text{z226}} \quad \mathbb{G}_3^{(c)}(B_{2g}, a) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{2}$$

$$\boxed{\text{z227}} \quad \mathbb{G}_3^{(c)}(B_{2g}, b) = \frac{3\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{10} - \frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{5} - \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{5} + \frac{3\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{10} - \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{5} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{5}$$

$$\boxed{\text{z228}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) = -\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z229}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2}$$

$$\boxed{\text{z230}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, c) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{4} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{4} + \frac{\sqrt{3}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z231}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, d) = \mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_3^{(b)}(B_{1u})$$

$$\boxed{\text{z232}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, e) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2}$$

$$\boxed{\text{z233}} \quad \mathbb{G}_4^{(c)}(B_{2u}) = \frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{4} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{4} + \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$$\boxed{\text{z234}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{2}$$

$$\boxed{\text{z235}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{2}$$

$$\boxed{\text{z236}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z237}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z238}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, c) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_4^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z239}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, c) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_4^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z240}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, d) = -\frac{\sqrt{78}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{26} - \frac{\sqrt{78}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{26} + \frac{\sqrt{78}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{26} + \frac{\sqrt{78}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{26} + \frac{\sqrt{26}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{26}$$

$$\boxed{\text{z241}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, d) = \frac{\sqrt{78}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{26} + \frac{\sqrt{78}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{26} + \frac{\sqrt{78}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{26} + \frac{\sqrt{78}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{26} + \frac{\sqrt{26}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{26}$$

$$\boxed{\text{z242}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, e) = -\frac{\sqrt{742}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_4^{(b)}(B_{2g})}{53} + \frac{5\sqrt{106}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_4^{(b)}(B_{2g})}{106}$$

$$\boxed{\text{z243}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, e) = -\frac{\sqrt{742}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_4^{(b)}(B_{2g})}{53} + \frac{5\sqrt{106}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_4^{(b)}(B_{2g})}{106}$$

$$\boxed{\text{z346}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{1g}, f) = \frac{\sqrt{30}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{48} - \frac{\sqrt{15}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{12} - \frac{\sqrt{30}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{48} + \frac{\sqrt{15}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{12} \\ - \frac{\sqrt{3}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} + \frac{\sqrt{210}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{48} + \frac{\sqrt{210}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{48}$$

$$\boxed{\text{z347}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{1g}, f) = -\frac{\sqrt{30}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{48} + \frac{\sqrt{15}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{12} - \frac{\sqrt{30}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{48} \\ + \frac{\sqrt{15}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{12} - \frac{\sqrt{3}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{210}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{48} + \frac{\sqrt{210}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{48}$$

$$\boxed{\text{z348}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, a) = \frac{\sqrt{26}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{52} + \frac{\sqrt{26}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{52} - \frac{\sqrt{26}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{52} - \frac{\sqrt{26}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{52} + \frac{\sqrt{78}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{13}$$

$$\boxed{\text{z349}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, a) = -\frac{\sqrt{26}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{52} - \frac{\sqrt{26}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{52} - \frac{\sqrt{26}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{52} - \frac{\sqrt{26}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{52} + \frac{\sqrt{78}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{13}$$

$$\boxed{\text{z350}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z351}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z352}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, c) = \frac{5\sqrt{106}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_4^{(b)}(B_{2g})}{106} + \frac{\sqrt{742}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_4^{(b)}(B_{2g})}{53}$$

$$\boxed{\text{z353}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, c) = \frac{5\sqrt{106}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_4^{(b)}(B_{2g})}{106} + \frac{\sqrt{742}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_4^{(b)}(B_{2g})}{53}$$

$$\boxed{\text{z354}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{1g}, d) = -\frac{125\sqrt{2274}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{18192} - \frac{43\sqrt{1137}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{4548} + \frac{125\sqrt{2274}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{18192} \\ + \frac{43\sqrt{1137}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{4548} + \frac{\sqrt{5685}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{2274} - \frac{29\sqrt{15918}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{18192} - \frac{29\sqrt{15918}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{18192}$$

$$\boxed{\text{z355}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{1g}, d) = \frac{125\sqrt{2274}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{18192} + \frac{43\sqrt{1137}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{4548} + \frac{125\sqrt{2274}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{18192} \\ + \frac{43\sqrt{1137}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{4548} + \frac{\sqrt{5685}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{2274} + \frac{29\sqrt{15918}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{18192} - \frac{29\sqrt{15918}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{18192}$$

$$\boxed{\text{z356}} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 1) = \frac{\sqrt{3}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} - \frac{\sqrt{3}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{6}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6}$$

$$\boxed{\text{z357}} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 1) = -\frac{\sqrt{3}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{3}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} + \frac{\sqrt{6}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6}$$

$$\boxed{\text{z358}} \quad \mathbb{Q}_{6,1}^{(c)}(E_{1g}, 2) = \frac{\sqrt{2653}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{758} - \frac{2\sqrt{5306}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{1137} - \frac{\sqrt{2653}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{758} + \frac{2\sqrt{5306}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{1137} \\ + \frac{3\sqrt{26530}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{758} + \frac{17\sqrt{379}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2274} + \frac{17\sqrt{379}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2274}$$

$$\boxed{\text{z359}} \quad \mathbb{Q}_{6,2}^{(c)}(E_{1g}, 2) = -\frac{\sqrt{2653}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{758} + \frac{2\sqrt{5306}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{1137} - \frac{\sqrt{2653}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{758} + \frac{2\sqrt{5306}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{1137} \\ + \frac{3\sqrt{26530}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{758} - \frac{17\sqrt{379}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2274} + \frac{17\sqrt{379}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2274}$$

$$\boxed{\text{z360}} \quad \mathbb{G}_{1,1}^{(c)}(E_{1g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{4} - \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{4} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{4} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{4}$$

$$\boxed{\text{z361}} \quad \mathbb{G}_{1,2}^{(c)}(E_{1g}) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{4} + \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{4} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{4} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{4}$$

$$\boxed{\text{z362}} \quad \mathbb{G}_{3,1}^{(c)}(E_{1g}) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{4} - \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{4} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{12} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{12}$$

$$\boxed{\text{z363}} \quad \mathbb{G}_{3,2}^{(c)}(E_{1g}) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{4} + \frac{\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{4} + \frac{\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} + \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{12} - \frac{\sqrt{14}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{12}$$

$$\boxed{\text{z364}} \quad \mathbb{G}_{5,1}^{(c)}(E_{1g}, 1) = \frac{\sqrt{6}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} - \frac{\sqrt{6}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} + \frac{\sqrt{3}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6} - \frac{\sqrt{3}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6}$$

$$\boxed{\text{z365}} \quad \mathbb{G}_{5,2}^{(c)}(E_{1g}, 1) = -\frac{\sqrt{6}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{6}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} - \frac{\sqrt{3}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6} - \frac{\sqrt{3}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6}$$

$$\boxed{\text{z366}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, a) = \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z367}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, a) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z368}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, b) = \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2}$$

$$\boxed{\text{z369}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, b) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2}$$

$$\boxed{\text{z370}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, c) = -\frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z371}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, c) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{\text{z372}} \quad \mathbb{Q}_{1,1}^{(c)}(E_{1u}, d) = -\frac{\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{8} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{8} - \frac{\sqrt{15}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{8} + \frac{\sqrt{15}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{8}$$

$$\boxed{\text{z373}} \quad \mathbb{Q}_{1,2}^{(c)}(E_{1u}, d) = \frac{\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{8} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{8} + \frac{\sqrt{15}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{8} + \frac{\sqrt{15}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{8}$$

$$\boxed{\text{z374}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, a) = -\frac{\sqrt{15}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{12} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{12} - \frac{\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z375}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, a) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{12} + \frac{\sqrt{15}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{12} + \frac{\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z398}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{1u}, b) = \frac{\sqrt{15}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{8} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{8} - \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{8} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{8}$$

$$\boxed{\text{z399}} \quad \mathbb{Q}_{3,2}^{(c)}(E_{1u}, b) = -\frac{\sqrt{15}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{8} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{8} + \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{8} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{8}$$

$$\boxed{\text{z400}} \quad \mathbb{Q}_{5,1}^{(c)}(E_{1u}, 1) = \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2}$$

$$\boxed{\text{z401}} \quad \mathbb{Q}_{5,2}^{(c)}(E_{1u}, 1) = -\frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2}$$

$$\boxed{\text{z402}} \quad \mathbb{G}_{2,1}^{(c)}(E_{1u}, a) = \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z403}} \quad \mathbb{G}_{2,2}^{(c)}(E_{1u}, a) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{\text{z426}} \quad \mathbb{G}_{2,1}^{(c)}(E_{1u}, b) = \frac{\sqrt{210}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{42} + \frac{2\sqrt{21}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{21} - \frac{\sqrt{210}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{42} - \frac{\sqrt{14}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{14}$$

$$\boxed{\text{z427}} \quad \mathbb{G}_{2,2}^{(c)}(E_{1u}, b) = -\frac{2\sqrt{21}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{21} - \frac{\sqrt{210}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{42} - \frac{\sqrt{210}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{42} + \frac{\sqrt{14}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{14}$$

$$\boxed{\text{z428}} \quad \mathbb{G}_{4,1}^{(c)}(E_{1u}) = -\frac{\sqrt{21}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{28} + \frac{\sqrt{210}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{28} + \frac{\sqrt{21}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{28} + \frac{\sqrt{35}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{14}$$

$$\boxed{\text{z429}} \quad \mathbb{G}_{4,2}^{(c)}(E_{1u}) = -\frac{\sqrt{210}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{28} + \frac{\sqrt{21}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{28} + \frac{\sqrt{21}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{28} - \frac{\sqrt{35}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{14}$$

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

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

$$\boxed{\text{z463}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z464}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z485}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, c) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_4^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z486}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, c) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_4^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z487}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, d) = -\frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{10} + \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{10} - \frac{\sqrt{5}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{5}$$

$$\boxed{\text{z488}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, d) = \frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{10} + \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{10} - \frac{\sqrt{5}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{5}$$

$$\boxed{\text{z489}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, e) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_4^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z490}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, e) = -\frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_4^{(b)}(B_{2g})}{2}$$

$$\boxed{\text{z593}} \quad \mathbb{Q}_{2,1}^{(c)}(E_{2g}, f) = \frac{\sqrt{555}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{222} + \frac{\sqrt{7770}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{222} - \frac{\sqrt{555}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{222} - \frac{\sqrt{7770}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{222} \\ + \frac{\sqrt{222}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{222} - \frac{\sqrt{3885}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{222} + \frac{\sqrt{3885}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{222}$$

$$\boxed{\text{z594}} \quad \mathbb{Q}_{2,2}^{(c)}(E_{2g}, f) = -\frac{\sqrt{555}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{222} - \frac{\sqrt{7770}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{222} - \frac{\sqrt{555}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{222} \\ - \frac{\sqrt{7770}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{222} + \frac{\sqrt{222}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{222} + \frac{\sqrt{3885}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{222} + \frac{\sqrt{3885}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{222}$$

$$\boxed{\text{z595}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1a) = \frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z596}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1a) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2}$$

$$\boxed{\text{z597}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1b) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z598}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1b) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z599}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 1c) = -\frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6}$$

$$\boxed{\text{z600}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 1c) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6} + \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} - \frac{\sqrt{7}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6}$$

$$\boxed{\text{z601}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2a) = -\frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{10} + \frac{\sqrt{30}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{10}$$

$$\boxed{\text{z602}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2a) = \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{10} + \frac{\sqrt{30}\mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{10}$$

$$\boxed{\text{z603}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2b) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z604}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2b) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z605}} \quad \mathbb{Q}_{4,1}^{(c)}(E_{2g}, 2c) = -\frac{137\sqrt{30747}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{122988} - \frac{13\sqrt{430458}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{61494} + \frac{137\sqrt{30747}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{122988} \\ + \frac{13\sqrt{430458}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{61494} - \frac{47\sqrt{307470}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{61494} - \frac{85\sqrt{215229}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{122988} + \frac{85\sqrt{215229}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{122988}$$

$$\boxed{\text{z606}} \quad \mathbb{Q}_{4,2}^{(c)}(E_{2g}, 2c) = \frac{137\sqrt{30747}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{122988} + \frac{13\sqrt{430458}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{61494} + \frac{137\sqrt{30747}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{122988} + \frac{13\sqrt{430458}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{61494} \\ - \frac{47\sqrt{307470}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{61494} + \frac{85\sqrt{215229}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{122988} + \frac{85\sqrt{215229}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{122988}$$

$$\boxed{\text{z607}} \quad \mathbb{Q}_{6,1}^{(c)}(E_{2g}, 1) = \frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6} - \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6}$$

$$\boxed{\text{z608}} \quad \mathbb{Q}_{6,2}^{(c)}(E_{2g}, 1) = -\frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{6} - \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{6} + \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{6} - \frac{\sqrt{2}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{6}$$

$$\boxed{\text{z609}} \quad \mathbb{Q}_{6,1}^{(c)}(E_{2g}, 2) = -\frac{17\sqrt{11634}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{4155} + \frac{11\sqrt{831}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2770} + \frac{17\sqrt{11634}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{4155} \\ - \frac{11\sqrt{831}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2770} + \frac{7\sqrt{29085}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{4155} + \frac{\sqrt{1662}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{1385} - \frac{\sqrt{1662}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{1385}$$

$$\boxed{\text{z610}} \quad \mathbb{Q}_{6,2}^{(c)}(E_{2g}, 2) = \frac{17\sqrt{11634}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{4155} - \frac{11\sqrt{831}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{2770} + \frac{17\sqrt{11634}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{4155} \\ - \frac{11\sqrt{831}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{2770} + \frac{7\sqrt{29085}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{4155} - \frac{\sqrt{1662}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{1385} - \frac{\sqrt{1662}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{1385}$$

$$\boxed{\text{z611}} \quad \mathbb{G}_{3,1}^{(c)}(E_{2g}) = -\frac{\sqrt{21}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{60} + \frac{\sqrt{6}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{10} + \frac{\sqrt{21}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{60} - \frac{\sqrt{6}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{10} \\ - \frac{\sqrt{210}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{30} + \frac{3\sqrt{3}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{20} - \frac{3\sqrt{3}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{20}$$

$$\boxed{\text{z612}} \quad \mathbb{G}_{3,2}^{(c)}(E_{2g}) = \frac{\sqrt{21}\mathbb{Q}_{4,1}^{(a)}(E_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{60} - \frac{\sqrt{6}\mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{10} + \frac{\sqrt{21}\mathbb{Q}_{4,2}^{(a)}(E_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{60} - \frac{\sqrt{6}\mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1)\mathbb{Q}_{2,1}^{(b)}(E_{2g})}{10} \\ - \frac{\sqrt{210}\mathbb{Q}_4^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_{2g})}{30} - \frac{3\sqrt{3}\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_{1g})}{20} - \frac{3\sqrt{3}\mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{1g})}{20}$$

$$\boxed{\text{z701}} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, a) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{z702} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{z703} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, b) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2}$$

$$\boxed{z704} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, b) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2}$$

$$\boxed{z705} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, c) = \frac{\sqrt{15}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{12} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{12} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{6} + \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{4} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{4}$$

$$\boxed{z706} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, c) = -\frac{\sqrt{15}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{12} + \frac{\sqrt{6}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{6} - \frac{\sqrt{15}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{12} - \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{4} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{4}$$

$$\boxed{z707} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, d) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{z708} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, d) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_3^{(b)}(B_{1u})}{2}$$

$$\boxed{z709} \quad \mathbb{Q}_{3,1}^{(c)}(E_{2u}, e) = \frac{\sqrt{2}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2}$$

$$\boxed{z710} \quad \mathbb{Q}_{3,2}^{(c)}(E_{2u}, e) = -\frac{\sqrt{2}\mathbb{M}_3^{(a)}(A_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2}$$

$$\boxed{z711} \quad \mathbb{Q}_{5,1}^{(c)}(E_{2u}, 1) = -\frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2}$$

$$\boxed{z712} \quad \mathbb{Q}_{5,2}^{(c)}(E_{2u}, 1) = \frac{\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{M}_{2,2}^{(b)}(E_{2u})}{2} + \frac{\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{M}_{2,1}^{(b)}(E_{2u})}{2}$$

$$\boxed{z713} \quad \mathbb{G}_{2,1}^{(c)}(E_{2u}, a) = \frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{z714} \quad \mathbb{G}_{2,2}^{(c)}(E_{2u}, a) = -\frac{\mathbb{M}_{1,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{z715} \quad \mathbb{G}_{2,1}^{(c)}(E_{2u}, b) = -\frac{\sqrt{21}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{42} + \frac{\sqrt{21}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{42} + \frac{\sqrt{210}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{42} + \frac{\sqrt{35}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{14} + \frac{\sqrt{35}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{14}$$

$$\boxed{z716} \quad \mathbb{G}_{2,2}^{(c)}(E_{2u}, b) = \frac{\sqrt{21}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{42} - \frac{\sqrt{210}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{42} + \frac{\sqrt{21}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{42} - \frac{\sqrt{35}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{14} + \frac{\sqrt{35}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{14}$$

$$\boxed{z717} \quad \mathbb{G}_{4,1}^{(c)}(E_{2u}, 1) = -\frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2}$$

$$\boxed{z718} \quad \mathbb{G}_{4,2}^{(c)}(E_{2u}, 1) = \frac{\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{2} + \frac{\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{2}$$

$$\boxed{z719} \quad \mathbb{G}_{4,1}^{(c)}(E_{2u}, 2) = \frac{\sqrt{105}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{28} - \frac{\sqrt{105}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{28} + \frac{\sqrt{42}\mathbb{M}_{3,2}^{(a)}(E_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{14} - \frac{\sqrt{7}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{28} - \frac{\sqrt{7}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{28}$$

$$\boxed{z720} \quad \mathbb{G}_{4,2}^{(c)}(E_{2u}, 2) = -\frac{\sqrt{105}\mathbb{M}_{3,1}^{(a)}(E_{1g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{28} - \frac{\sqrt{42}\mathbb{M}_{3,1}^{(a)}(E_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{14} - \frac{\sqrt{105}\mathbb{M}_{3,2}^{(a)}(E_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{28} + \frac{\sqrt{7}\mathbb{M}_3^{(a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_{1u})}{28} - \frac{\sqrt{7}\mathbb{M}_3^{(a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_{1u})}{28}$$

Atomic SAMB

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

$$\boxed{x1} \quad \mathbb{Q}_0^{(a)}(A_{1g}) = \begin{bmatrix} \frac{\sqrt{5}}{5} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{5}}{5} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{5}}{5} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{5}}{5} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{5}}{5} \end{bmatrix}$$

$$\boxed{x2} \quad \mathbb{Q}_2^{(a)}(A_{1g}) = \begin{bmatrix} -\frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{14} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{7} \end{bmatrix}$$

$$\boxed{x3} \quad \mathbb{Q}_4^{(a)}(A_{1g}) = \begin{bmatrix} \frac{\sqrt{70}}{70} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{70}}{70} & 0 & 0 & 0 \\ 0 & 0 & -\frac{2\sqrt{70}}{35} & 0 & 0 \\ 0 & 0 & 0 & -\frac{2\sqrt{70}}{35} & 0 \\ 0 & 0 & 0 & 0 & \frac{3\sqrt{70}}{35} \end{bmatrix}$$

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

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

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

$$\boxed{x7} \quad \mathbb{Q}_{2,2}^{(a)}(E_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{14} & 0 \\ -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & -\frac{\sqrt{14}}{14} \\ 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{14}}{14} & 0 & 0 \end{bmatrix}$$

$$\boxed{x8} \quad \mathbb{Q}_{4,1}^{(a)}(E_{1g}) = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{7}}{14} & 0 \\ 0 & 0 & -\frac{\sqrt{7}}{14} & 0 & 0 \\ 0 & -\frac{\sqrt{7}}{14} & 0 & 0 & 0 \\ \frac{\sqrt{7}}{14} & 0 & 0 & 0 & \frac{\sqrt{21}}{7} \\ 0 & 0 & 0 & \frac{\sqrt{21}}{7} & 0 \end{bmatrix}$$

$$\boxed{x9} \quad \mathbb{Q}_{4,2}^{(a)}(E_{1g}) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{7}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{7}}{14} & 0 \\ \frac{\sqrt{7}}{14} & 0 & 0 & 0 & -\frac{\sqrt{21}}{7} \\ 0 & \frac{\sqrt{7}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{21}}{7} & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{x12} \quad \mathbb{Q}_{4,1}^{(a)}(E_{2g}, 1) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x13} \quad \mathbb{Q}_{4,2}^{(a)}(E_{2g}, 1) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x14} \quad \mathbb{Q}_{4,1}^{(a)}(E_{2g}, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{14}}{7} & 0 \\ \frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x15} \quad \mathbb{Q}_{4,2}^{(a)}(E_{2g}, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & -\frac{\sqrt{14}}{7} & 0 \\ 0 & 0 & -\frac{\sqrt{14}}{7} & 0 & 0 \\ 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x16} \quad \mathbb{M}_1^{(a)}(A_{2g}) = \begin{bmatrix} 0 & -\frac{\sqrt{10i}}{5} & 0 & 0 & 0 \\ \frac{\sqrt{10i}}{5} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10i}}{10} & 0 \\ 0 & 0 & \frac{\sqrt{10i}}{10} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x17} \quad \mathbb{M}_3^{(a)}(A_{2g}) = \begin{bmatrix} 0 & \frac{\sqrt{10i}}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{10i}}{10} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{10i}}{5} & 0 \\ 0 & 0 & \frac{\sqrt{10i}}{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x18} \quad \mathbb{M}_3^{(a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & \frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} & 0 \\ -\frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x19} \quad \mathbb{M}_3^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & -\frac{i}{2} & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x20} \quad \mathbb{M}_{1,1}^{(a)}(E_{1g}) = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & \frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & -\frac{\sqrt{30}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{30}i}{10} & 0 \end{bmatrix}$$

$$\boxed{x21} \quad \mathbb{M}_{1,2}^{(a)}(E_{1g}) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{10}i}{10} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{10} & 0 \\ -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 & \frac{\sqrt{30}i}{10} \\ 0 & -\frac{\sqrt{10}i}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{30}i}{10} & 0 & 0 \end{bmatrix}$$

$$\boxed{x22} \quad \mathbb{M}_{3,1}^{(a)}(E_{1g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{10} & 0 & 0 \\ 0 & -\frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & -\frac{\sqrt{5}i}{5} \\ 0 & 0 & 0 & \frac{\sqrt{5}i}{5} & 0 \end{bmatrix}$$

$$\boxed{x23} \quad \mathbb{M}_{3,2}^{(a)}(E_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{15}i}{10} & 0 \\ \frac{\sqrt{15}i}{10} & 0 & 0 & 0 & \frac{\sqrt{5}i}{5} \\ 0 & \frac{\sqrt{15}i}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{5}i}{5} & 0 & 0 \end{bmatrix}$$

$$\boxed{x24} \quad \mathbb{M}_{3,1}^{(a)}(E_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x25} \quad \mathbb{M}_{3,2}^{(a)}(E_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{2} & 0 & 0 & 0 \end{bmatrix}$$

— Cluster SAMB —

- Site cluster

** Wyckoff: 2c

$$\boxed{y1} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2} \right]$$

$$\boxed{y2} \quad \mathbb{Q}_3^{(s)}(B_{1u}) = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

** Wyckoff: 6h

$$\boxed{y3} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y4}} \quad \mathbb{Q}_3^{(s)}(B_{1u}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y5}} \quad \mathbb{Q}_{1,1}^{(s)}(E_{1u}) = \left[0, -\frac{1}{2}, \frac{1}{2}, 0, \frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{\text{y6}} \quad \mathbb{Q}_{1,2}^{(s)}(E_{1u}) = \left[\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6} \right]$$

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

$$\boxed{\text{y8}} \quad \mathbb{Q}_{2,2}^{(s)}(E_{2g}) = \left[0, \frac{1}{2}, -\frac{1}{2}, 0, \frac{1}{2}, -\frac{1}{2} \right]$$

• Bond cluster

** Wyckoff: **6b@6h**

$$\boxed{\text{y9}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y10}} \quad \mathbb{M}_1^{(s)}(A_{2g}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y11}} \quad \mathbb{Q}_3^{(s)}(B_{1u}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y12}} \quad \mathbb{T}_3^{(s)}(B_{2u}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6} \right]$$

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

$$\boxed{\text{y14}} \quad \mathbb{Q}_{1,2}^{(s)}(E_{1u}) = \left[\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y15}} \quad \mathbb{T}_{1,1}^{(s)}(E_{1u}) = \left[\frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y16}} \quad \mathbb{T}_{1,2}^{(s)}(E_{1u}) = \left[0, \frac{i}{2}, -\frac{i}{2}, 0, -\frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{\text{y17}} \quad \mathbb{Q}_{2,1}^{(s)}(E_{2g}) = \left[\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y18}} \quad \mathbb{Q}_{2,2}^{(s)}(E_{2g}) = \left[0, \frac{1}{2}, -\frac{1}{2}, 0, \frac{1}{2}, -\frac{1}{2} \right]$$

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

$$\boxed{\text{y20}} \quad \mathbb{T}_{2,2}^{(s)}(E_{2g}) = \left[-\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6} \right]$$

** Wyckoff: **6a@6g**

$$\boxed{\text{y21}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y22}} \quad \mathbb{T}_1^{(s)}(A_{2u}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y23}} \quad \mathbb{T}_3^{(s)}(B_{1u}) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y24}} \quad \mathbb{Q}_4^{(s)}(B_{2g}) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y25}} \quad \mathbb{Q}_{2,1}^{(s)}(E_{1g}) = \left[\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6} \right]$$

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

$$\boxed{\text{y27}} \quad \mathbb{T}_{1,1}^{(s)}(E_{1u}) = \left[0, -\frac{i}{2}, \frac{i}{2}, 0, \frac{i}{2}, -\frac{i}{2} \right]$$

$$\boxed{\text{y28}} \quad \mathbb{T}_{1,2}^{(s)}(E_{1u}) = \left[\frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y29}} \quad \mathbb{Q}_{2,1}^{(s)}(E_{2g}) = \left[\frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y30}} \quad \mathbb{Q}_{2,2}^{(s)}(E_{2g}) = \left[0, \frac{1}{2}, -\frac{1}{2}, 0, \frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{\text{y31}} \quad \mathbb{M}_{2,1}^{(s)}(E_{2u}) = \left[0, -\frac{i}{2}, \frac{i}{2}, 0, -\frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{\text{y32}} \quad \mathbb{M}_{2,2}^{(s)}(E_{2u}) = \left[\frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{3}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6} \right]$$

** Wyckoff: 12a@12j

$$\boxed{\text{y33}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y34}} \quad \mathbb{T}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y35}} \quad \mathbb{M}_1^{(s)}(A_{2g}) = \left[\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y36}} \quad \mathbb{Q}_6^{(s)}(A_{2g}) = \left[\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y37}} \quad \mathbb{Q}_3^{(s)}(B_{1u}) = \left[\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y38}} \quad \mathbb{T}_3^{(s)}(B_{1u}) = \left[\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y39}} \quad \mathbb{Q}_3^{(s)}(B_{2u}) = \left[\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6} \right]$$

$$\boxed{\text{y40}} \quad \mathbb{T}_3^{(s)}(B_{2u}) = \left[\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, \frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6}, -\frac{\sqrt{3}i}{6} \right]$$

$$\boxed{\text{y41}} \quad \mathbb{Q}_{1,1}^{(s)}(E_{1u}) = \left[\frac{5\sqrt{42}}{84}, -\frac{\sqrt{42}}{21}, -\frac{\sqrt{42}}{84}, -\frac{5\sqrt{42}}{84}, \frac{\sqrt{42}}{21}, \frac{\sqrt{42}}{84}, -\frac{\sqrt{42}}{84}, \frac{5\sqrt{42}}{84}, -\frac{\sqrt{42}}{21}, \frac{\sqrt{42}}{84}, -\frac{5\sqrt{42}}{84}, \frac{\sqrt{42}}{21} \right]$$

$$\boxed{\text{y42}} \quad \mathbb{Q}_{1,2}^{(s)}(E_{1u}) = \left[\frac{\sqrt{14}}{28}, \frac{\sqrt{14}}{14}, -\frac{3\sqrt{14}}{28}, -\frac{\sqrt{14}}{28}, -\frac{\sqrt{14}}{14}, \frac{3\sqrt{14}}{28}, \frac{3\sqrt{14}}{28}, -\frac{\sqrt{14}}{28}, -\frac{\sqrt{14}}{14}, -\frac{3\sqrt{14}}{28}, \frac{\sqrt{14}}{28}, \frac{\sqrt{14}}{14} \right]$$

$$\boxed{\text{y43}} \quad \mathbb{T}_{1,1}^{(s)}(E_{1u}, a) = \left[\frac{5\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{21}, -\frac{\sqrt{42}i}{84}, -\frac{5\sqrt{42}i}{84}, \frac{\sqrt{42}i}{21}, \frac{\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{84}, \frac{5\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{21}, \frac{\sqrt{42}i}{84}, -\frac{5\sqrt{42}i}{84}, \frac{\sqrt{42}i}{21} \right]$$

$$\boxed{\text{y44}} \quad \mathbb{T}_{1,2}^{(s)}(E_{1u}, a) = \left[\frac{\sqrt{14}i}{28}, \frac{\sqrt{14}i}{14}, -\frac{3\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{14}, \frac{3\sqrt{14}i}{28}, \frac{3\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{14}, -\frac{3\sqrt{14}i}{28}, \frac{\sqrt{14}i}{28}, \frac{\sqrt{14}i}{14} \right]$$

$$\boxed{\text{y45}} \quad \mathbb{T}_{1,1}^{(s)}(E_{1u}, b) = \left[\frac{\sqrt{14}i}{28}, \frac{\sqrt{14}i}{14}, -\frac{3\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{14}, \frac{3\sqrt{14}i}{28}, -\frac{3\sqrt{14}i}{28}, \frac{\sqrt{14}i}{28}, \frac{\sqrt{14}i}{14}, \frac{3\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{28}, -\frac{\sqrt{14}i}{14} \right]$$

$$\boxed{\text{y46}} \quad \mathbb{T}_{1,2}^{(s)}(E_{1u}, b) = \left[-\frac{5\sqrt{42}i}{84}, \frac{\sqrt{42}i}{21}, \frac{\sqrt{42}i}{84}, \frac{5\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{21}, -\frac{\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{84}, \frac{5\sqrt{42}i}{84}, -\frac{\sqrt{42}i}{21}, \frac{\sqrt{42}i}{84}, -\frac{5\sqrt{42}i}{84}, \frac{\sqrt{42}i}{21} \right]$$

$$\boxed{\text{y47}} \quad \mathbb{Q}_{5,1}^{(s)}(E_{1u}, 1) = \left[\frac{\sqrt{14}}{28}, \frac{\sqrt{14}}{14}, -\frac{3\sqrt{14}}{28}, -\frac{\sqrt{14}}{28}, -\frac{\sqrt{14}}{14}, \frac{3\sqrt{14}}{28}, -\frac{3\sqrt{14}}{28}, \frac{\sqrt{14}}{28}, \frac{\sqrt{14}}{14}, \frac{3\sqrt{14}}{28}, -\frac{\sqrt{14}}{28}, -\frac{\sqrt{14}}{14} \right]$$

$$\boxed{\text{y48}} \quad \mathbb{Q}_{5,2}^{(s)}(E_{1u}, 1) = \left[-\frac{5\sqrt{42}}{84}, \frac{\sqrt{42}}{21}, \frac{\sqrt{42}}{84}, \frac{5\sqrt{42}}{84}, -\frac{\sqrt{42}}{21}, -\frac{\sqrt{42}}{84}, -\frac{\sqrt{42}}{84}, \frac{5\sqrt{42}}{84}, -\frac{\sqrt{42}}{21}, \frac{\sqrt{42}}{84}, -\frac{5\sqrt{42}}{84}, \frac{\sqrt{42}}{21} \right]$$

$$\boxed{\text{y49}} \quad \mathbb{Q}_{2,1}^{(s)}(E_{2g}) = \left[\frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42}, -\frac{13\sqrt{6}}{84}, \frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42}, -\frac{13\sqrt{6}}{84}, -\frac{13\sqrt{6}}{84}, \frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42}, -\frac{13\sqrt{6}}{84}, \frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42} \right]$$

$$\boxed{\text{y50}} \quad \mathbb{Q}_{2,2}^{(s)}(E_{2g}) = \left[-\frac{5\sqrt{2}}{28}, \frac{2\sqrt{2}}{7}, -\frac{3\sqrt{2}}{28}, -\frac{5\sqrt{2}}{28}, \frac{2\sqrt{2}}{7}, -\frac{3\sqrt{2}}{28}, \frac{3\sqrt{2}}{28}, \frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7}, \frac{3\sqrt{2}}{28}, \frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7} \right]$$

$$\boxed{\text{y51}} \quad \mathbb{T}_{2,1}^{(s)}(E_{2g}, a) = \left[\frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42}, -\frac{13\sqrt{6}i}{84}, \frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42}, -\frac{13\sqrt{6}i}{84}, -\frac{13\sqrt{6}i}{84}, \frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42}, -\frac{13\sqrt{6}i}{84}, \frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42} \right]$$

$$\boxed{\text{y52}} \quad \mathbb{T}_{2,2}^{(s)}(E_{2g}, a) = \left[-\frac{5\sqrt{2}i}{28}, \frac{2\sqrt{2}i}{7}, -\frac{3\sqrt{2}i}{28}, -\frac{5\sqrt{2}i}{28}, \frac{2\sqrt{2}i}{7}, -\frac{3\sqrt{2}i}{28}, \frac{3\sqrt{2}i}{28}, \frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7}, \frac{3\sqrt{2}i}{28}, \frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7} \right]$$

$$\boxed{\text{y53}} \quad \mathbb{T}_{2,1}^{(s)}(E_{2g}, b) = \left[\frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7}, \frac{3\sqrt{2}i}{28}, \frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7}, \frac{3\sqrt{2}i}{28}, \frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7}, \frac{3\sqrt{2}i}{28}, \frac{5\sqrt{2}i}{28}, -\frac{2\sqrt{2}i}{7} \right]$$

$$\boxed{y54} \quad \mathbb{T}_{2,2}^{(s)}(E_{2g}, b) = \left[\frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42}, -\frac{13\sqrt{6}i}{84}, \frac{11\sqrt{6}i}{84}, \frac{\sqrt{6}i}{42}, -\frac{13\sqrt{6}i}{84}, \frac{13\sqrt{6}i}{84}, -\frac{11\sqrt{6}i}{84}, -\frac{\sqrt{6}i}{42}, \frac{13\sqrt{6}i}{84}, -\frac{11\sqrt{6}i}{84}, -\frac{\sqrt{6}i}{42} \right]$$

$$\boxed{y55} \quad \mathbb{Q}_{4,1}^{(s)}(E_{2g}, 1) = \left[\frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7}, \frac{3\sqrt{2}}{28}, \frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7}, \frac{3\sqrt{2}}{28}, \frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7}, \frac{3\sqrt{2}}{28}, \frac{5\sqrt{2}}{28}, -\frac{2\sqrt{2}}{7} \right]$$

$$\boxed{y56} \quad \mathbb{Q}_{4,2}^{(s)}(E_{2g}, 1) = \left[\frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42}, -\frac{13\sqrt{6}}{84}, \frac{11\sqrt{6}}{84}, \frac{\sqrt{6}}{42}, -\frac{13\sqrt{6}}{84}, \frac{13\sqrt{6}}{84}, -\frac{11\sqrt{6}}{84}, -\frac{\sqrt{6}}{42}, \frac{13\sqrt{6}}{84}, -\frac{11\sqrt{6}}{84}, -\frac{\sqrt{6}}{42} \right]$$

— Site and Bond —

Table 5: Orbital of each site

| # | site | orbital |
|---|------|--|
| 1 | Mn | $ d_v\rangle, d_{xy}\rangle, d_{xz}\rangle, d_{yz}\rangle, d_u\rangle$ |
| 2 | Sn | $ d_v\rangle, d_{xy}\rangle, d_{xz}\rangle, d_{yz}\rangle, d_u\rangle$ |

Table 6: Neighbor and bra-ket of each bond

| # | head | tail | neighbor | head (bra) | tail (ket) |
|---|------|------|----------|------------|------------|
| 1 | Mn | Mn | [1] | [d] | [d] |
| 2 | Mn | Sn | [1] | [d] | [d] |
| 3 | Sn | Sn | [1] | [d] | [d] |

— Site in Unit Cell —

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

Table 7: 'Mn' (#1) site cluster (6h), mm2

| SL | position (<i>s</i>) | mapping |
|----|------------------------------|--------------|
| 1 | [0.83880, 0.67760, 0.25000] | [1,11,16,20] |
| 2 | [0.32240, 0.16120, 0.25000] | [2,10,17,19] |
| 3 | [0.83880, 0.16120, 0.25000] | [3,12,18,21] |
| 4 | [0.16120, 0.32240, 0.75000] | [4,8,13,23] |
| 5 | [0.67760, 0.83880, 0.75000] | [5,7,14,22] |
| 6 | [0.16120, 0.83880, 0.75000] | [6,9,15,24] |

Table 8: 'Sn' (#2) site cluster (2c), -6m2

| SL | position (<i>s</i>) | mapping |
|----|------------------------------|------------------------------------|
| 1 | [0.33333, 0.66667, 0.25000] | [1,2,3,10,11,12,16,17,18,19,20,21] |
| 2 | [0.66667, 0.33333, 0.75000] | [4,5,6,7,8,9,13,14,15,22,23,24] |

Bond in Unit Cell

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

Table 9: 1-th 'Mn'-'Mn' [1] (#1) bond cluster (6b@6h), ND, $|v|=0.4836$ (cartesian)

| SL | vector (v) | center (c) | mapping | head | tail | R (primitive) |
|----|------------------------------|------------------------------|----------------|-------|-------|-----------------|
| 1 | [-0.48360, 0.00000, 0.00000] | [0.08060, 0.16120, 0.25000] | [1,-11,16,-20] | (3,1) | (2,1) | [1,0,0] |
| 2 | [0.00000,-0.48360, 0.00000] | [0.83880, 0.91940, 0.25000] | [2,-10,17,-19] | (1,1) | (3,1) | [0,1,0] |
| 3 | [0.48360, 0.48360, 0.00000] | [0.08060, 0.91940, 0.25000] | [3,-12,18,-21] | (2,1) | (1,1) | [-1,-1,0] |
| 4 | [0.48360, 0.00000, 0.00000] | [0.91940, 0.83880, 0.75000] | [4,-8,13,-23] | (6,1) | (5,1) | [-1,0,0] |
| 5 | [0.00000, 0.48360, 0.00000] | [0.16120, 0.08060, 0.75000] | [5,-7,14,-22] | (4,1) | (6,1) | [0,-1,0] |
| 6 | [-0.48360,-0.48360, 0.00000] | [0.91940, 0.08060, 0.75000] | [6,-9,15,-24] | (5,1) | (4,1) | [1,1,0] |

Table 10: 1-th 'Mn'-'Sn' [1] (#2) bond cluster (12a@12j), D, $|v|=0.50009$ (cartesian)

| SL | vector (v) | center (c) | mapping | head | tail | R (primitive) |
|----|------------------------------|------------------------------|---------|-------|-------|-----------------|
| 1 | [-0.49453, 0.01093, 0.00000] | [0.08607, 0.67213, 0.25000] | [1,16] | (1,1) | (1,1) | [1,0,0] |
| 2 | [-0.01093,-0.50547, 0.00000] | [0.32787, 0.41393, 0.25000] | [2,17] | (2,1) | (1,1) | [0,0,0] |
| 3 | [0.50547, 0.49453, 0.00000] | [0.58607, 0.91393, 0.25000] | [3,18] | (3,1) | (1,1) | [0,-1,0] |
| 4 | [0.49453,-0.01093, 0.00000] | [0.91393, 0.32787, 0.75000] | [4,13] | (4,1) | (2,1) | [-1,0,0] |
| 5 | [0.01093, 0.50547, 0.00000] | [0.67213, 0.58607, 0.75000] | [5,14] | (5,1) | (2,1) | [0,0,0] |
| 6 | [-0.50547,-0.49453, 0.00000] | [0.41393, 0.08607, 0.75000] | [6,15] | (6,1) | (2,1) | [0,1,0] |
| 7 | [0.01093,-0.49453, 0.00000] | [0.67213, 0.08607, 0.75000] | [7,22] | (5,1) | (2,1) | [0,1,0] |
| 8 | [-0.50547,-0.01093, 0.00000] | [0.41393, 0.32787, 0.75000] | [8,23] | (4,1) | (2,1) | [0,0,0] |
| 9 | [0.49453, 0.50547, 0.00000] | [0.91393, 0.58607, 0.75000] | [9,24] | (6,1) | (2,1) | [-1,0,0] |

continued ...

Table 10

| SL | vector (v) | center (c) | mapping | head | tail | R (primitive) |
|----|---------------------------------|-------------------------------|---------|-------|-------|-----------------|
| 10 | [-0.01093, 0.49453, 0.00000] | [0.32787, 0.91393, 0.25000] | [10,19] | (2,1) | (1,1) | [0,-1,0] |
| 11 | [0.50547, 0.01093, 0.00000] | [0.58607, 0.67213, 0.25000] | [11,20] | (1,1) | (1,1) | [0,0,0] |
| 12 | [-0.49453, -0.50547, 0.00000] | [0.08607, 0.41393, 0.25000] | [12,21] | (3,1) | (1,1) | [1,0,0] |

Table 11: 1-th 'Sn'-'Sn' [1] (#3) bond cluster (6a@6g), ND, $|v|=0.76376$ (cartesian)

| SL | vector (v) | center (c) | mapping | head | tail | R (primitive) |
|----|----------------------------------|-------------------------------|----------------|-------|-------|-----------------|
| 1 | [0.33333, 0.66667, -0.50000] | [0.50000, 0.00000, 0.00000] | [1,-8,-13,20] | (2,1) | (1,1) | [0,-1,1] |
| 2 | [-0.66667, -0.33333, -0.50000] | [0.00000, 0.50000, 0.00000] | [2,-7,-14,19] | (2,1) | (1,1) | [1,0,1] |
| 3 | [0.33333, -0.33333, -0.50000] | [0.50000, 0.50000, 0.00000] | [3,-9,-15,21] | (2,1) | (1,1) | [0,0,1] |
| 4 | [-0.33333, -0.66667, -0.50000] | [0.50000, 0.00000, 0.50000] | [4,-11,-16,23] | (1,1) | (2,1) | [0,1,0] |
| 5 | [0.66667, 0.33333, -0.50000] | [0.00000, 0.50000, 0.50000] | [5,-10,-17,22] | (1,1) | (2,1) | [-1,0,0] |
| 6 | [-0.33333, 0.33333, -0.50000] | [0.50000, 0.50000, 0.50000] | [6,-12,-18,24] | (1,1) | (2,1) | [0,0,0] |