

Model for “UPt₂Si₂”

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

Group and Unit Cell

- Group: SG No. 129 D_{4h}⁷ P4/nmm [tetragonal]
- Associated point group: PG No. 129 D_{4h} 4/mmm [tetragonal]
- Unit cell:

$a = 4.19720, b = 4.19720, c = 9.69060, \alpha = 90.0, \beta = 90.0, \gamma = 90.0$
- Lattice vectors (conventional cell):

$\mathbf{a}_1 = [4.19720, 0.00000, 0.00000]$
 $\mathbf{a}_2 = [0.00000, 4.19720, 0.00000]$
 $\mathbf{a}_3 = [0.00000, 0.00000, 9.69060]$

Symmetry Operation

Table 1: Symmetry operation

| # | SO | # | SO | # | SO | # | SO | # | SO |
|----|---|----|---|----|--|----|--|----|---|
| 1 | {1 0} | 2 | {2001 $\frac{1}{2}\frac{1}{2}0$ } | 3 | {4 ⁺ ₀₀₁ $\frac{1}{2}00$ } | 4 | {4 ⁻ ₀₀₁ $0\frac{1}{2}0$ } | 5 | {2010 $0\frac{1}{2}0$ } |
| 6 | {2100 $\frac{1}{2}00$ } | 7 | {2110 $\frac{1}{2}\frac{1}{2}0$ } | 8 | {2 ₁₋₁₀ 0} | 9 | {-1 0} | 10 | {m ₀₀₁ $\frac{1}{2}\frac{1}{2}0$ } |
| 11 | {-4 ⁺ ₀₀₁ $\frac{1}{2}00$ } | 12 | {-4 ⁻ ₀₀₁ $0\frac{1}{2}0$ } | 13 | {m ₀₁₀ $0\frac{1}{2}0$ } | 14 | {m ₁₀₀ $\frac{1}{2}00$ } | 15 | {m ₁₁₀ $\frac{1}{2}\frac{1}{2}0$ } |
| 16 | {m ₁₋₁₀ 0} | | | | | | | | |

Harmonics

Table 2: Harmonics

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|---|---------------------------|----------|------|--------|--------------|-----------|---|
| 1 | $\mathbb{Q}_0(A_{1g})$ | A_{1g} | 0 | Q, T | - | - | 1 |
| 2 | $\mathbb{Q}_2(A_{1g})$ | A_{1g} | 2 | Q, T | - | - | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| 3 | $\mathbb{Q}_4(A_{1g}, 1)$ | A_{1g} | 4 | Q, T | 1 | - | $\frac{\sqrt{21}(x^4 - 3x^2y^2 - 3x^2z^2 + y^4 - 3y^2z^2 + z^4)}{6}$ |
| 4 | $\mathbb{Q}_4(A_{1g}, 2)$ | A_{1g} | 4 | Q, T | 2 | - | $-\frac{\sqrt{15}(x^4 - 12x^2y^2 + 6x^2z^2 + y^4 + 6y^2z^2 - 2z^4)}{12}$ |
| 5 | $\mathbb{G}_5(A_{1g})$ | A_{1g} | 5 | G, M | - | - | $\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$ |
| 6 | $\mathbb{Q}_6(A_{1g}, 1)$ | A_{1g} | 6 | Q, T | 1 | - | $\frac{\sqrt{2}(2x^6 - 15x^4y^2 - 15x^4z^2 - 15x^2y^4 + 180x^2y^2z^2 - 15x^2z^4 + 2y^6 - 15y^4z^2 - 15y^2z^4 + 2z^6)}{8}$ |

continued ...

Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|----|---------------------------|----------|------|--------|--------------|-----------|--|
| 7 | $\mathbb{Q}_6(A_{1g}, 2)$ | A_{1g} | 6 | Q, T | 2 | - | $-\frac{\sqrt{14}(x^6 - 15x^4z^2 + 15x^2z^4 + y^6 - 15y^4z^2 + 15y^2z^4 - 2z^6)}{8}$ |
| 8 | $\mathbb{G}_0(A_{1u})$ | A_{1u} | 0 | G, M | - | - | 1 |
| 9 | $\mathbb{G}_2(A_{1u})$ | A_{1u} | 2 | G, M | - | - | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| 10 | $\mathbb{G}_4(A_{1u}, 1)$ | A_{1u} | 4 | G, M | 1 | - | $\frac{\sqrt{21}(x^4 - 3x^2y^2 - 3x^2z^2 + y^4 - 3y^2z^2 + z^4)}{6}$ |
| 11 | $\mathbb{Q}_5(A_{1u})$ | A_{1u} | 5 | Q, T | - | - | $\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$ |
| 12 | $\mathbb{G}_1(A_{2g})$ | A_{2g} | 1 | G, M | - | - | z |
| 13 | $\mathbb{G}_3(A_{2g})$ | A_{2g} | 3 | G, M | - | - | $-\frac{z(3x^2 + 3y^2 - 2z^2)}{2}$ |
| 14 | $\mathbb{Q}_4(A_{2g})$ | A_{2g} | 4 | Q, T | - | - | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$ |
| 15 | $\mathbb{G}_5(A_{2g}, 1)$ | A_{2g} | 5 | G, M | 1 | - | $\frac{z(15x^4 + 30x^2y^2 - 40x^2z^2 + 15y^4 - 40y^2z^2 + 8z^4)}{8}$ |
| 16 | $\mathbb{G}_5(A_{2g}, 2)$ | A_{2g} | 5 | G, M | 2 | - | $\frac{3\sqrt{35}z(x^2 - 2xy - y^2)(x^2 + 2xy - y^2)}{8}$ |
| 17 | $\mathbb{Q}_6(A_{2g})$ | A_{2g} | 6 | Q, T | - | - | $-\frac{3\sqrt{7}xy(x-y)(x+y)(x^2 + y^2 - 10z^2)}{4}$ |
| 18 | $\mathbb{Q}_1(A_{2u})$ | A_{2u} | 1 | Q, T | - | - | z |
| 19 | $\mathbb{Q}_3(A_{2u})$ | A_{2u} | 3 | Q, T | - | - | $-\frac{z(3x^2 + 3y^2 - 2z^2)}{2}$ |
| 20 | $\mathbb{Q}_5(A_{2u}, 1)$ | A_{2u} | 5 | Q, T | 1 | - | $\frac{z(15x^4 + 30x^2y^2 - 40x^2z^2 + 15y^4 - 40y^2z^2 + 8z^4)}{8}$ |
| 21 | $\mathbb{Q}_5(A_{2u}, 2)$ | A_{2u} | 5 | Q, T | 2 | - | $\frac{3\sqrt{35}z(x^2 - 2xy - y^2)(x^2 + 2xy - y^2)}{8}$ |
| 22 | $\mathbb{Q}_2(B_{1g})$ | B_{1g} | 2 | Q, T | - | - | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| 23 | $\mathbb{G}_3(B_{1g})$ | B_{1g} | 3 | G, M | - | - | $\sqrt{15}xyz$ |
| 24 | $\mathbb{Q}_4(B_{1g})$ | B_{1g} | 4 | Q, T | - | - | $\frac{\sqrt{5}(x-y)(x+y)(x^2 + y^2 - 6z^2)}{4}$ |
| 25 | $\mathbb{G}_5(B_{1g})$ | B_{1g} | 5 | G, M | - | - | $\frac{\sqrt{105}xyz(x^2 + y^2 - 2z^2)}{2}$ |
| 26 | $\mathbb{Q}_6(B_{1g}, 1)$ | B_{1g} | 6 | Q, T | 1 | - | $-\frac{\sqrt{2310}(x-y)(x+y)(x-z)(x+z)(y-z)(y+z)}{8}$ |
| 27 | $\mathbb{Q}_6(B_{1g}, 2)$ | B_{1g} | 6 | Q, T | 2 | - | $\frac{\sqrt{42}(x-y)(x+y)(x^4 - 9x^2y^2 - 5x^2z^2 + y^4 - 5y^2z^2 + 5z^4)}{8}$ |

continued ...

Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|----|----------------------------|----------|------|--------|--------------|-----------|--|
| 28 | $\mathbb{G}_2(B_{1u})$ | B_{1u} | 2 | G, M | - | - | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| 29 | $\mathbb{Q}_3(B_{1u})$ | B_{1u} | 3 | Q, T | - | - | $\sqrt{15}xyz$ |
| 30 | $\mathbb{Q}_5(B_{1u})$ | B_{1u} | 5 | Q, T | - | - | $\frac{\sqrt{105}xyz(x^2+y^2-2z^2)}{2}$ |
| 31 | $\mathbb{Q}_7(B_{1u}, 1)$ | B_{1u} | 7 | Q, T | 1 | - | $\frac{\sqrt{91}xyz(3x^4-5x^2y^2-5x^2z^2+3y^4-5y^2z^2+3z^4)}{2}$ |
| 32 | $\mathbb{Q}_2(B_{2g})$ | B_{2g} | 2 | Q, T | - | - | $\sqrt{3}xy$ |
| 33 | $\mathbb{G}_3(B_{2g})$ | B_{2g} | 3 | G, M | - | - | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |
| 34 | $\mathbb{Q}_4(B_{2g})$ | B_{2g} | 4 | Q, T | - | - | $-\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$ |
| 35 | $\mathbb{G}_5(B_{2g})$ | B_{2g} | 5 | G, M | - | - | $-\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$ |
| 36 | $\mathbb{Q}_6(B_{2g}, 1)$ | B_{2g} | 6 | Q, T | 1 | - | $\frac{\sqrt{462}xy(x^2-3y^2)(3x^2-y^2)}{16}$ |
| 37 | $\mathbb{Q}_6(B_{2g}, 2)$ | B_{2g} | 6 | Q, T | 2 | - | $\frac{\sqrt{210}xy(x^4+2x^2y^2-16x^2z^2+y^4-16y^2z^2+16z^4)}{16}$ |
| 38 | $\mathbb{G}_2(B_{2u})$ | B_{2u} | 2 | G, M | - | - | $\sqrt{3}xy$ |
| 39 | $\mathbb{Q}_3(B_{2u})$ | B_{2u} | 3 | Q, T | - | - | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |
| 40 | $\mathbb{Q}_5(B_{2u})$ | B_{2u} | 5 | Q, T | - | - | $-\frac{\sqrt{105}z(x-y)(x+y)(x^2+y^2-2z^2)}{4}$ |
| 41 | $\mathbb{Q}_7(B_{2u}, 1)$ | B_{2u} | 7 | Q, T | 1 | - | $\frac{\sqrt{6006}z(x-y)(x+y)(x^2-4xy+y^2)(x^2+4xy+y^2)}{32}$ |
| 42 | $\mathbb{G}_{1,1}(E_g)$ | E_g | 1 | G, M | - | 1 | x |
| 43 | $\mathbb{G}_{1,2}(E_g)$ | | | | | 2 | $-y$ |
| 44 | $\mathbb{Q}_{2,1}(E_g)$ | E_g | 2 | Q, T | - | 1 | $\sqrt{3}yz$ |
| 45 | $\mathbb{Q}_{2,2}(E_g)$ | | | | | 2 | $\sqrt{3}xz$ |
| 46 | $\mathbb{G}_{3,1}(E_g, 1)$ | E_g | 3 | G, M | 1 | 1 | $\frac{x(2x^2-3y^2-3z^2)}{2}$ |
| 47 | $\mathbb{G}_{3,2}(E_g, 1)$ | | | | | 2 | $\frac{y(3x^2-2y^2+3z^2)}{2}$ |
| 48 | $\mathbb{G}_{3,1}(E_g, 2)$ | E_g | 3 | G, M | 2 | 1 | $\frac{\sqrt{15}x(y-z)(y+z)}{2}$ |

continued ...

Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|----|----------------------------|--------|------|--------|--------------|-----------|--|
| 49 | $\mathbb{G}_{3,2}(E_g, 2)$ | | | | | 2 | $-\frac{\sqrt{15}y(x-z)(x+z)}{2}$ |
| 50 | $\mathbb{Q}_{4,1}(E_g, 1)$ | E_g | 4 | Q, T | 1 | 1 | $\frac{\sqrt{35}yz(y-z)(y+z)}{2}$ |
| 51 | $\mathbb{Q}_{4,2}(E_g, 1)$ | | | | | 2 | $\frac{\sqrt{35}xz(x-z)(x+z)}{2}$ |
| 52 | $\mathbb{Q}_{4,1}(E_g, 2)$ | E_g | 4 | Q, T | 2 | 1 | $\frac{\sqrt{5}yz(6x^2-y^2-z^2)}{2}$ |
| 53 | $\mathbb{Q}_{4,2}(E_g, 2)$ | | | | | 2 | $-\frac{\sqrt{5}xz(x^2-6y^2+z^2)}{2}$ |
| 54 | $\mathbb{G}_{5,1}(E_g, 1)$ | E_g | 5 | G, M | 1 | 1 | $\frac{x(8x^4-40x^2y^2-40x^2z^2+15y^4+30y^2z^2+15z^4)}{8}$ |
| 55 | $\mathbb{G}_{5,2}(E_g, 1)$ | | | | | 2 | $-\frac{y(15x^4-40x^2y^2+30x^2z^2+8y^4-40y^2z^2+15z^4)}{8}$ |
| 56 | $\mathbb{G}_{5,1}(E_g, 2)$ | E_g | 5 | G, M | 2 | 1 | $\frac{3\sqrt{35}x(y^2-2yz-z^2)(y^2+2yz-z^2)}{8}$ |
| 57 | $\mathbb{G}_{5,2}(E_g, 2)$ | | | | | 2 | $-\frac{3\sqrt{35}y(x^2-2xz-z^2)(x^2+2xz-z^2)}{8}$ |
| 58 | $\mathbb{G}_{5,1}(E_g, 3)$ | E_g | 5 | G, M | 3 | 1 | $\frac{\sqrt{105}x(y-z)(y+z)(2x^2-y^2-z^2)}{4}$ |
| 59 | $\mathbb{G}_{5,2}(E_g, 3)$ | | | | | 2 | $\frac{\sqrt{105}y(x-z)(x+z)(x^2-2y^2+z^2)}{4}$ |
| 60 | $\mathbb{Q}_{6,1}(E_g, 1)$ | E_g | 6 | Q, T | 1 | 1 | $\frac{3\sqrt{7}yz(y-z)(y+z)(10x^2-y^2-z^2)}{4}$ |
| 61 | $\mathbb{Q}_{6,2}(E_g, 1)$ | | | | | 2 | $-\frac{3\sqrt{7}xz(x-z)(x+z)(x^2-10y^2+z^2)}{4}$ |
| 62 | $\mathbb{Q}_{6,1}(E_g, 2)$ | E_g | 6 | Q, T | 2 | 1 | $\frac{\sqrt{462}yz(y^2-3z^2)(3y^2-z^2)}{16}$ |
| 63 | $\mathbb{Q}_{6,2}(E_g, 2)$ | | | | | 2 | $\frac{\sqrt{462}xz(x^2-3z^2)(3x^2-z^2)}{16}$ |
| 64 | $\mathbb{Q}_{6,1}(E_g, 3)$ | E_g | 6 | Q, T | 3 | 1 | $\frac{\sqrt{210}yz(16x^4-16x^2y^2-16x^2z^2+y^4+2y^2z^2+z^4)}{16}$ |
| 65 | $\mathbb{Q}_{6,2}(E_g, 3)$ | | | | | 2 | $\frac{\sqrt{210}xz(x^4-16x^2y^2+2x^2z^2+16y^4-16y^2z^2+z^4)}{16}$ |
| 66 | $\mathbb{Q}_{1,1}(E_u)$ | E_u | 1 | Q, T | - | 1 | x |
| 67 | $\mathbb{Q}_{1,2}(E_u)$ | | | | | 2 | y |
| 68 | $\mathbb{G}_{2,1}(E_u)$ | E_u | 2 | G, M | - | 1 | $\sqrt{3}yz$ |
| 69 | $\mathbb{G}_{2,2}(E_u)$ | | | | | 2 | $-\sqrt{3}xz$ |

continued ...

Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|----|----------------------------|--------|------|--------|--------------|-----------|--|
| 70 | $\mathbb{Q}_{3,1}(E_u, 1)$ | E_u | 3 | Q, T | 1 | 1 | $\frac{x(2x^2 - 3y^2 - 3z^2)}{2}$ |
| 71 | $\mathbb{Q}_{3,2}(E_u, 1)$ | | | | | 2 | $-\frac{y(3x^2 - 2y^2 + 3z^2)}{2}$ |
| 72 | $\mathbb{Q}_{3,1}(E_u, 2)$ | E_u | 3 | Q, T | 2 | 1 | $\frac{\sqrt{15}x(y-z)(y+z)}{2}$ |
| 73 | $\mathbb{Q}_{3,2}(E_u, 2)$ | | | | | 2 | $\frac{\sqrt{15}y(x-z)(x+z)}{2}$ |
| 74 | $\mathbb{Q}_{5,1}(E_u, 1)$ | E_u | 5 | Q, T | 1 | 1 | $\frac{x(8x^4 - 40x^2y^2 - 40x^2z^2 + 15y^4 + 30y^2z^2 + 15z^4)}{8}$ |
| 75 | $\mathbb{Q}_{5,2}(E_u, 1)$ | | | | | 2 | $\frac{y(15x^4 - 40x^2y^2 + 30x^2z^2 + 8y^4 - 40y^2z^2 + 15z^4)}{8}$ |
| 76 | $\mathbb{Q}_{5,1}(E_u, 2)$ | E_u | 5 | Q, T | 2 | 1 | $\frac{3\sqrt{35}x(y^2 - 2yz - z^2)(y^2 + 2yz - z^2)}{8}$ |
| 77 | $\mathbb{Q}_{5,2}(E_u, 2)$ | | | | | 2 | $\frac{3\sqrt{35}y(x^2 - 2xz - z^2)(x^2 + 2xz - z^2)}{8}$ |
| 78 | $\mathbb{Q}_{5,1}(E_u, 3)$ | E_u | 5 | Q, T | 3 | 1 | $\frac{\sqrt{105}x(y-z)(y+z)(2x^2 - y^2 - z^2)}{4}$ |
| 79 | $\mathbb{Q}_{5,2}(E_u, 3)$ | | | | | 2 | $-\frac{\sqrt{105}y(x-z)(x+z)(x^2 - 2y^2 + z^2)}{4}$ |

Basis in full matrix

Table 3: dimension = 46

| # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) |
|----|-----------------------|----|-----------------------|----|--------------------------|----|--------------------------|----|--------------------------|
| 0 | $ d_u\rangle @Pt1(1)$ | 1 | $ d_v\rangle @Pt1(1)$ | 2 | $ d_{yz}\rangle @Pt1(1)$ | 3 | $ d_{xz}\rangle @Pt1(1)$ | 4 | $ d_{xy}\rangle @Pt1(1)$ |
| 5 | $ d_u\rangle @Pt1(2)$ | 6 | $ d_v\rangle @Pt1(2)$ | 7 | $ d_{yz}\rangle @Pt1(2)$ | 8 | $ d_{xz}\rangle @Pt1(2)$ | 9 | $ d_{xy}\rangle @Pt1(2)$ |
| 10 | $ d_u\rangle @Pt2(1)$ | 11 | $ d_v\rangle @Pt2(1)$ | 12 | $ d_{yz}\rangle @Pt2(1)$ | 13 | $ d_{xz}\rangle @Pt2(1)$ | 14 | $ d_{xy}\rangle @Pt2(1)$ |

continued ...

Table 3

| # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) |
|----|------------------------|----|------------------------|----|--------------------------|----|--------------------------|----|--------------------------|
| 15 | $ d_u\rangle @Pt2(2)$ | 16 | $ d_v\rangle @Pt2(2)$ | 17 | $ d_{yz}\rangle @Pt2(2)$ | 18 | $ d_{xz}\rangle @Pt2(2)$ | 19 | $ d_{xy}\rangle @Pt2(2)$ |
| 20 | $ p_x\rangle @Si1(1)$ | 21 | $ p_y\rangle @Si1(1)$ | 22 | $ p_z\rangle @Si1(1)$ | 23 | $ p_x\rangle @Si1(2)$ | 24 | $ p_y\rangle @Si1(2)$ |
| 25 | $ p_z\rangle @Si1(2)$ | 26 | $ p_x\rangle @Si2(1)$ | 27 | $ p_y\rangle @Si2(1)$ | 28 | $ p_z\rangle @Si2(1)$ | 29 | $ p_x\rangle @Si2(2)$ |
| 30 | $ p_y\rangle @Si2(2)$ | 31 | $ p_z\rangle @Si2(2)$ | 32 | $ f_3\rangle @U(1)$ | 33 | $ f_{ax}\rangle @U(1)$ | 34 | $ f_{ay}\rangle @U(1)$ |
| 35 | $ f_{az}\rangle @U(1)$ | 36 | $ f_{bx}\rangle @U(1)$ | 37 | $ f_{by}\rangle @U(1)$ | 38 | $ f_{bz}\rangle @U(1)$ | 39 | $ f_3\rangle @U(2)$ |
| 40 | $ f_{ax}\rangle @U(2)$ | 41 | $ f_{ay}\rangle @U(2)$ | 42 | $ f_{az}\rangle @U(2)$ | 43 | $ f_{bx}\rangle @U(2)$ | 44 | $ f_{by}\rangle @U(2)$ |
| 45 | $ f_{bz}\rangle @U(2)$ | | | | | | | | |

Table 4: Atomic basis (orbital part only)

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

continued ...

Table 4

| orbital | definition |
|----------------|----------------------------------|
| $ f_3\rangle$ | $\sqrt{15}xyz$ |
| $ fax\rangle$ | $\frac{x(2x^2-3y^2-3z^2)}{2}$ |
| $ fay\rangle$ | $\frac{y(-3x^2+2y^2-3z^2)}{2}$ |
| $ fa_z\rangle$ | $\frac{z(-3x^2-3y^2+2z^2)}{2}$ |
| $ fb_x\rangle$ | $\frac{\sqrt{15}x(y^2-z^2)}{2}$ |
| $ fb_y\rangle$ | $\frac{\sqrt{15}y(-x^2+z^2)}{2}$ |
| $ fb_z\rangle$ | $\frac{\sqrt{15}z(x^2-y^2)}{2}$ |

SAMB

380 (all 380) SAMBs

- 'Pt1' site-cluster : Pt1
 - * bra: $\langle d_u |$, $\langle d_v |$, $\langle d_{yz} |$, $\langle d_{xz} |$, $\langle d_{xy} |$
 - * ket: $|d_u \rangle$, $|d_v \rangle$, $|d_{yz} \rangle$, $|d_{xz} \rangle$, $|d_{xy} \rangle$
 - * wyckoff: 2a

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

[z2] $\mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$

[z3] $\mathbb{Q}_4^{(c)}(A_{1g}, 1) = \mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})$

[z4] $\mathbb{Q}_4^{(c)}(A_{1g}, 2) = \mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})$

[z35] $\mathbb{Q}_5^{(c)}(A_{1u}, a) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_3^{(s)}(B_{2u})$

$$\boxed{\text{z53}} \quad \mathbb{Q}_5^{(c)}(A_{1u}, b) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z54}} \quad \mathbb{Q}_4^{(c)}(A_{2g}) = \mathbb{Q}_4^{(a)}(A_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z79}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z80}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = -\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z103}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z104}} \quad \mathbb{Q}_4^{(c)}(B_{1g}) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z105}} \quad \mathbb{Q}_3^{(c)}(B_{1u}) = \mathbb{Q}_4^{(a)}(A_{2g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z106}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z107}} \quad \mathbb{Q}_4^{(c)}(B_{2g}) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z108}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z191}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) = -\frac{\mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_3^{(s)}(B_{2u})}{6} - \frac{\sqrt{35}\mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_3^{(s)}(B_{2u})}{6}$$

$$\boxed{\text{z192}} \quad \mathbb{Q}_5^{(c)}(B_{2u}, a) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z211}} \quad \mathbb{Q}_5^{(c)}(B_{2u}, b) = -\frac{\sqrt{35}\mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_3^{(s)}(B_{2u})}{6} + \frac{\mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_3^{(s)}(B_{2u})}{6}$$

$$\boxed{\text{z212}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z242}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z264}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

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

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

$$\boxed{\text{z267}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z293}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_3^{(s)}(B_{2u})}{2}$$

$$\boxed{\text{z294}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_3^{(s)}(B_{2u})}{2}$$

$$\boxed{\text{z295}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, b) = \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_3^{(s)}(B_{2u})}{8} - \frac{3\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_3^{(s)}(B_{2u})}{8}$$

$$\boxed{\text{z296}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, b) = -\frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_3^{(s)}(B_{2u})}{8} + \frac{3\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_3^{(s)}(B_{2u})}{8}$$

$$\boxed{\text{z297}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1) = \frac{3\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_3^{(s)}(B_{2u})}{8} + \frac{\sqrt{14}\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_3^{(s)}(B_{2u})}{8}$$

$$\boxed{\text{z298}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1) = -\frac{3\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_3^{(s)}(B_{2u})}{8} - \frac{\sqrt{14}\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_3^{(s)}(B_{2u})}{8}$$

• 'Pt2' site-cluster : Pt2

- * bra: $\langle d_u |, \langle d_v |, \langle d_{yz} |, \langle d_{xz} |, \langle d_{xy} |$
- * ket: $|d_u \rangle, |d_v \rangle, |d_{yz} \rangle, |d_{xz} \rangle, |d_{xy} \rangle$
- * wyckoff: 2c

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

$$\boxed{\text{z6}} \quad \mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z7}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 1) = \mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z8}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 2) = \mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z36}} \quad \mathbb{Q}_5^{(c)}(A_{1u}) = \mathbb{Q}_4^{(a)}(A_{2g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z55}} \quad \mathbb{Q}_4^{(c)}(A_{2g}) = \mathbb{Q}_4^{(a)}(A_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z56}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z81}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z82}} \quad \mathbb{Q}_3^{(c)}(A_{2u}) = \frac{\sqrt{21}\mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{6} + \frac{\sqrt{15}\mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{6}$$

$$\boxed{\text{z109}} \quad \mathbb{Q}_5^{(c)}(A_{2u}, 2) = \frac{\sqrt{15}\mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{6} - \frac{\sqrt{21}\mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{6}$$

$$\boxed{\text{z110}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z111}} \quad \mathbb{Q}_4^{(c)}(B_{1g}) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z112}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z113}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_1^{(s)}(A_{2u})$$

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

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

$$\boxed{\text{z213}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z214}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) = -\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z215}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z216}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z243}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z244}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z268}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z269}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z299}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_1^{(s)}(A_{2u})}{2}$$

$$\boxed{\text{z300}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_1^{(s)}(A_{2u})}{2}$$

$$\boxed{\text{z301}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1) = \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z302}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1) = \frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} - \frac{\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z303}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2) = \frac{\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z304}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

- 'Si1' site-cluster : **Si1**
 - * bra: $\langle p_x |, \langle p_y |, \langle p_z |$
 - * ket: $|p_x\rangle, |p_y\rangle, |p_z\rangle$
 - * wyckoff: 2b

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

$$\boxed{\text{z10}} \quad \mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z57}} \quad \mathbb{Q}_5^{(c)}(A_{1u}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z83}} \quad \mathbb{Q}_1^{(c)}(A_{2u}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_3^{(s)}(B_{2u})$$

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

$$\boxed{\text{z116}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z194}} \quad \mathbb{Q}_3^{(c)}(B_{2u}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{2u})$$

$$\boxed{\text{z217}} \quad \mathbb{Q}_5^{(c)}(B_{2u}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_3^{(s)}(B_{2u})$$

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

$$\boxed{\text{z271}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z305}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_3^{(s)}(B_{2u})}{2}$$

$$\boxed{\text{z306}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_3^{(s)}(B_{2u})}{2}$$

• 'Si2' site-cluster : **Si2**

- * bra: $\langle p_x |, \langle p_y |, \langle p_z |$
- * ket: $|p_x \rangle, |p_y \rangle, |p_z \rangle$
- * wyckoff: 2c

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

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

$$\boxed{\text{z58}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z84}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z117}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z118}} \quad \mathbb{Q}_3^{(c)}(B_{1u}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z218}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z219}} \quad \mathbb{Q}_3^{(c)}(B_{2u}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z245}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z272}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z307}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_1^{(s)}(A_{2u})}{2}$$

$$\boxed{\text{z308}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_1^{(s)}(A_{2u})}{2}$$

- 'U' site-cluster : U
- * bra: $\langle f_3|, \langle f_{ax}|, \langle f_{ay}|, \langle f_{az}|, \langle f_{bx}|, \langle f_{by}|, \langle f_{bz}|$
- * ket: $|f_3\rangle, |f_{ax}\rangle, |f_{ay}\rangle, |f_{az}\rangle, |f_{bx}\rangle, |f_{by}\rangle, |f_{bz}\rangle$
- * wyckoff: 2c

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

$$\boxed{\text{z14}} \quad \mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z15}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 1) = \mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z16}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 2) = \mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z17}} \quad \mathbb{Q}_6^{(c)}(A_{1g}, 1) = \mathbb{Q}_6^{(a)}(A_{1g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z18}} \quad \mathbb{Q}_6^{(c)}(A_{1g}, 2) = \mathbb{Q}_6^{(a)}(A_{1g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z37}} \quad \mathbb{Q}_5^{(c)}(A_{1u}, a) = \mathbb{Q}_4^{(a)}(A_{2g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z38}} \quad \mathbb{Q}_5^{(c)}(A_{1u}, b) = \mathbb{Q}_6^{(a)}(A_{2g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z59}} \quad \mathbb{Q}_4^{(c)}(A_{2g}) = \mathbb{Q}_4^{(a)}(A_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

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

$$\boxed{\text{z61}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z62}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z85}} \quad \mathbb{Q}_3^{(c)}(A_{2u}) = \frac{\sqrt{21}\mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{6} + \frac{\sqrt{15}\mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{6}$$

$$\boxed{\text{z86}} \quad \mathbb{Q}_5^{(c)}(A_{2u}, 1) = \frac{\sqrt{2}\mathbb{Q}_6^{(a)}(A_{1g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{14}\mathbb{Q}_6^{(a)}(A_{1g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z87}} \quad \mathbb{Q}_5^{(c)}(A_{2u}, 2a) = \frac{\sqrt{15}\mathbb{Q}_4^{(a)}(A_{1g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{6} - \frac{\sqrt{21}\mathbb{Q}_4^{(a)}(A_{1g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{6}$$

$$\boxed{\text{z88}} \quad \mathbb{Q}_5^{(c)}(A_{2u}, 2b) = -\frac{\sqrt{14}\mathbb{Q}_6^{(a)}(A_{1g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{2}\mathbb{Q}_6^{(a)}(A_{1g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z119}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z120}} \quad \mathbb{Q}_4^{(c)}(B_{1g}) = \mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z121}} \quad \mathbb{Q}_6^{(c)}(B_{1g}, 1) = \mathbb{Q}_6^{(a)}(B_{1g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z122}} \quad \mathbb{Q}_6^{(c)}(B_{1g}, 2) = \mathbb{Q}_6^{(a)}(B_{1g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z123}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z124}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z125}} \quad \mathbb{Q}_5^{(c)}(B_{1u}) = -\mathbb{Q}_6^{(a)}(B_{2g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z126}} \quad \mathbb{Q}_7^{(c)}(B_{1u}, 1) = \mathbb{Q}_6^{(a)}(B_{2g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z127}} \quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z128}} \quad \mathbb{Q}_4^{(c)}(B_{2g}) = \mathbb{Q}_4^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z129}} \quad \mathbb{Q}_6^{(c)}(B_{2g}, 1) = \mathbb{Q}_6^{(a)}(B_{2g}, 1)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z130}} \quad \mathbb{Q}_6^{(c)}(B_{2g}, 2) = \mathbb{Q}_6^{(a)}(B_{2g}, 2)\mathbb{Q}_0^{(s)}(A_{1g})$$

$$\boxed{\text{z195}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z196}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) = -\mathbb{Q}_4^{(a)}(B_{1g})\mathbb{Q}_1^{(s)}(A_{2u})$$

$$\boxed{\text{z220}} \quad \mathbb{Q}_5^{(c)}(B_{2u}) = -\frac{\sqrt{11}\mathbb{Q}_6^{(a)}(B_{1g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{5}\mathbb{Q}_6^{(a)}(B_{1g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z221}} \quad \mathbb{Q}_7^{(c)}(B_{2u}, 1) = \frac{\sqrt{5}\mathbb{Q}_6^{(a)}(B_{1g}, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{11}\mathbb{Q}_6^{(a)}(B_{1g}, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z222}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z223}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z224}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z225}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z246}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z247}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 2) = \frac{\sqrt{2}\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z248}} \quad \mathbb{Q}_{6,1}^{(c)}(E_g, 1) = \frac{\sqrt{2}\mathbb{Q}_{6,1}^{(a)}(E_g, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z249}} \quad \mathbb{Q}_{6,2}^{(c)}(E_g, 1) = \frac{\sqrt{2}\mathbb{Q}_{6,2}^{(a)}(E_g, 1)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z273}} \quad \mathbb{Q}_{6,1}^{(c)}(E_g, 2) = \frac{\sqrt{2}\mathbb{Q}_{6,1}^{(a)}(E_g, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z274}} \quad \mathbb{Q}_{6,2}^{(c)}(E_g, 2) = \frac{\sqrt{2}\mathbb{Q}_{6,2}^{(a)}(E_g, 2)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z275}} \quad \mathbb{Q}_{6,1}^{(c)}(E_g, 3) = \frac{\sqrt{2}\mathbb{Q}_{6,1}^{(a)}(E_g, 3)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z276}} \quad \mathbb{Q}_{6,2}^{(c)}(E_g, 3) = \frac{\sqrt{2}\mathbb{Q}_{6,2}^{(a)}(E_g, 3)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z309}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_1^{(s)}(A_{2u})}{2}$$

$$\boxed{\text{z310}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_1^{(s)}(A_{2u})}{2}$$

$$\boxed{\text{z311}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1) = \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} - \frac{\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z312}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1) = \frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} - \frac{\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z313}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2) = \frac{\mathbb{Q}_{4,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{7}\mathbb{Q}_{4,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z314}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2) = \frac{\mathbb{Q}_{4,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{4} + \frac{\sqrt{7}\mathbb{Q}_{4,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{4}$$

$$\boxed{\text{z315}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 1) = -\frac{\sqrt{6}\mathbb{Q}_{6,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{8} + \frac{3\sqrt{11}\mathbb{Q}_{6,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{16} + \frac{\sqrt{5}\mathbb{Q}_{6,2}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{16}$$

$$\boxed{\text{z316}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 1) = -\frac{\sqrt{6}\mathbb{Q}_{6,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{8} + \frac{3\sqrt{11}\mathbb{Q}_{6,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{16} + \frac{\sqrt{5}\mathbb{Q}_{6,1}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{16}$$

$$\boxed{\text{z317}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 2) = \frac{7\sqrt{290}\mathbb{Q}_{6,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{232} + \frac{\sqrt{4785}\mathbb{Q}_{6,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{464} + \frac{23\sqrt{87}\mathbb{Q}_{6,2}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{464}$$

$$\boxed{\text{z318}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 2) = \frac{7\sqrt{290}\mathbb{Q}_{6,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{232} + \frac{\sqrt{4785}\mathbb{Q}_{6,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{464} + \frac{23\sqrt{87}\mathbb{Q}_{6,1}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{464}$$

$$\boxed{\text{z319}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 3) = \frac{\sqrt{1914}\mathbb{Q}_{6,2}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{116} + \frac{13\sqrt{29}\mathbb{Q}_{6,2}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{232} - \frac{3\sqrt{1595}\mathbb{Q}_{6,2}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{232}$$

$$\boxed{\text{z320}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 3) = \frac{\sqrt{1914}\mathbb{Q}_{6,1}^{(a)}(E_g, 1)\mathbb{Q}_1^{(s)}(A_{2u})}{116} + \frac{13\sqrt{29}\mathbb{Q}_{6,1}^{(a)}(E_g, 2)\mathbb{Q}_1^{(s)}(A_{2u})}{232} - \frac{3\sqrt{1595}\mathbb{Q}_{6,1}^{(a)}(E_g, 3)\mathbb{Q}_1^{(s)}(A_{2u})}{232}$$

- 'Pt1'-'Si2' bond-cluster : Si2;Pt1_001_1

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

- * ket: $|p_x\rangle, |p_y\rangle, |p_z\rangle$

- * wyckoff: 8a@8i

$$\boxed{\text{z27}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, a) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z28}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z29}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, a) = -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z30}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, b) = -\frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z31}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, c) = -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z32}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, d) = -\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z33}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 1) = \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z34}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 2) = -\frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{42} + \frac{3\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{42} + \frac{3\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{21}$$

$$\boxed{\text{z46}} \quad \mathbb{Q}_5^{(c)}(A_{1u}) = \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{7}$$

$$\boxed{\text{z47}} \quad \mathbb{G}_0^{(c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z48}} \quad \mathbb{G}_2^{(c)}(A_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z49}} \quad \mathbb{G}_2^{(c)}(A_{1u}, b) = -\frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{5\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{84} + \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{5\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{84} - \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

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

$$\boxed{\text{z51}} \quad \mathbb{G}_2^{(c)}(A_{1u}, d) = \frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z52}} \quad \mathbb{G}_4^{(c)}(A_{1u}, 1) = -\frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z71}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, a) = \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z72}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, b) = \mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z73}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, c) = -\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_3^{(b)}(B_{2u})$$

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

$$\boxed{\text{z75}} \quad \mathbb{G}_1^{(c)}(A_{2g}, b) = \frac{\sqrt{30}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{5}$$

$$\boxed{\text{z76}} \quad \mathbb{G}_3^{(c)}(A_{2g}, a) = -\frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z77}} \quad \mathbb{G}_3^{(c)}(A_{2g}, b) = -\frac{\sqrt{5}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{5} + \frac{\sqrt{5}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{5}$$

$$\boxed{\text{z78}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z96}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z97}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, c) = -\frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} - \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{21} - \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} - \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z98}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, d) = -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z99}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, a) = \mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z100}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, b) = -\frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} - \frac{5\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{84} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{5\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{84} - \frac{4\sqrt{21}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z101}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, c) = -\frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z102}} \quad \mathbb{Q}_5^{(c)}(A_{2u}, 2) = \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4}$$

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

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

$$\boxed{\text{z163}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, c) = \frac{3\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{42} - \frac{3\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{42} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{21}$$

$$\boxed{\text{z164}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, d) = -\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z165}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, e) = -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z166}} \quad \mathbb{Q}_4^{(c)}(B_{1g}) = \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z167}} \quad \mathbb{G}_3^{(c)}(B_{1g}, a) = -\frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z168}} \quad \mathbb{G}_3^{(c)}(B_{1g}, b) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z169}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z170}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) = \mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z171}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, c) = -\frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z172}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, d) = \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z173}} \quad \mathbb{Q}_5^{(c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z174}} \quad \mathbb{G}_2^{(c)}(B_{1u}, a) = \mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z175}} \quad \mathbb{G}_2^{(c)}(B_{1u}, b) = -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z176}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z177}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, b) = -\frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{7} + \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{21} - \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{7} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{21} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{21}$$

$$\boxed{\text{z178}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, c) = -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z179}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, d) = \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z180}} \quad \mathbb{Q}_4^{(c)}(B_{2g}) = -\frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{28} - \frac{3\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{28} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{28} - \frac{3\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{28} + \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z181}} \quad \mathbb{G}_3^{(c)}(B_{2g}, a) = \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z182}} \quad \mathbb{G}_3^{(c)}(B_{2g}, b) = -\frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z183}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z184}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) = \mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z185}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, c) = \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} - \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z186}} \quad \mathbb{Q}_5^{(c)}(B_{2u}) = -\frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{21} - \frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} + \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z187}} \quad \mathbb{G}_2^{(c)}(B_{2u}, a) = -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z188}} \quad \mathbb{G}_2^{(c)}(B_{2u}, b) = -\frac{3\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{3\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{7}$$

$$\boxed{\text{z189}} \quad \mathbb{G}_2^{(c)}(B_{2u}, c) = \mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z190}} \quad \mathbb{G}_2^{(c)}(B_{2u}, d) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z204}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z205}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z206}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z207}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z208}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, c) = -\frac{\sqrt{14}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{14} - \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{42} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{42} - \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{42}$$

$$\boxed{\text{z209}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, c) = -\frac{\sqrt{14}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{14} - \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{42} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{42} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{42}$$

$$\boxed{\text{z210}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, d) = -\frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} + \frac{\sqrt{30}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z234}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, d) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} - \frac{\sqrt{30}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

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

$$\boxed{\text{z236}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, e) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} - \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z237}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1a) = \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z238}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1a) = \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z239}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1b) = -\frac{\sqrt{30}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z240}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1b) = \frac{\sqrt{30}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z241}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1c) = -\frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z257}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1c) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z258}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 2) = -\frac{\sqrt{70}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{56} + \frac{3\sqrt{42}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{56} - \frac{\sqrt{70}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{56} + \frac{\sqrt{42}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{3\sqrt{42}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{56}$$

$$\boxed{\text{z259}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 2) = -\frac{\sqrt{70}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{56} + \frac{3\sqrt{42}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{56} - \frac{\sqrt{70}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{56} + \frac{\sqrt{42}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{3\sqrt{42}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{56}$$

$$\boxed{\text{z260}} \quad \mathbb{G}_{1,1}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z261}} \quad \mathbb{G}_{1,2}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z262}} \quad \mathbb{G}_{1,1}^{(c)}(E_g, b) = -\frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z263}} \quad \mathbb{G}_{1,2}^{(c)}(E_g, b) = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z285}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 1a) = -\frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z286}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 1a) = -\frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z287}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 1b) = \frac{\sqrt{10}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{30}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{20} - \frac{\sqrt{10}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z288}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 1b) = \frac{\sqrt{10}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{30}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{20} + \frac{\sqrt{10}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z289}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 2a) = \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{24} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{24}$$

$$\boxed{\text{z290}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 2a) = \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{24} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{24}$$

$$\boxed{\text{z291}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 2b) = \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} - \frac{\sqrt{2}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z292}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 2b) = \frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} + \frac{\sqrt{2}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{12} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6}$$

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

$$\boxed{\text{z352}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z353}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, b) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z354}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, b) = -\frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z355}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, c) = \frac{3\sqrt{14}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{28} - \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{84} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{42}$$

$$\boxed{\text{z356}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, c) = -\frac{3\sqrt{14}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{28} + \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{84} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{42} - \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42}$$

$$\boxed{\text{z357}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, d) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{6} - \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z358}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, d) = -\frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{6} + \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z359}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1a) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z360}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1a) = -\frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z361}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1b) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z362}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1b) = \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z363}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1c) = \frac{33\sqrt{1834}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{3668} + \frac{17\sqrt{27510}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{11004} - \frac{2\sqrt{1834}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{917} - \frac{17\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5502} + \frac{2\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2751}$$

$$\boxed{\text{z364}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1c) = -\frac{33\sqrt{1834}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{3668} - \frac{17\sqrt{27510}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{11004} - \frac{2\sqrt{1834}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{917} - \frac{17\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{5502} - \frac{2\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2751}$$

$$\boxed{\text{z365}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1d) = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{30} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z366}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1d) = \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{30} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z367}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2a) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z368}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2a) = \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z369}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2b) = \frac{25\sqrt{655}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} - \frac{5\sqrt{393}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} - \frac{7\sqrt{655}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{1048} + \frac{5\sqrt{393}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{1048} - \frac{4\sqrt{393}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{131}$$

$$\boxed{\text{z370}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2b) = -\frac{25\sqrt{655}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} + \frac{5\sqrt{393}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} - \frac{7\sqrt{655}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{1048} + \frac{5\sqrt{393}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{1048} + \frac{4\sqrt{393}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{131}$$

$$\boxed{\text{z371}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2c) = \frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{10} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z372}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2c) = -\frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z373}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 1) = \frac{5\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{16} - \frac{\sqrt{15}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{80} + \frac{5\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{8} + \frac{\sqrt{15}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{40}$$

$$\boxed{\text{z374}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 1) = -\frac{5\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{16} + \frac{\sqrt{15}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{80} + \frac{5\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{8} + \frac{\sqrt{15}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{40}$$

$$\boxed{\text{z375}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 2) = -\frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{5} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z376}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 2) = \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{5} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z377}} \quad \mathbb{G}_{2,1}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z378}} \quad \mathbb{G}_{2,2}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z379}} \quad \mathbb{G}_{2,1}^{(c)}(E_u, b) = -\frac{\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z380}} \quad \mathbb{G}_{2,2}^{(c)}(E_u, b) = \frac{\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

• 'Pt2'-'Si1' bond-cluster : Si1;Pt2_001_1

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

* ket: $|p_x\rangle$, $|p_y\rangle$, $|p_z\rangle$

* wyckoff: 8a@8i

$$\boxed{\text{z19}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, a) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z20}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z21}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, a) = -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z22}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, b) = -\frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z23}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, c) = -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z24}} \quad \mathbb{Q}_2^{(c)}(A_{1g}, d) = -\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z25}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 1) = \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z26}} \quad \mathbb{Q}_4^{(c)}(A_{1g}, 2) = -\frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{42} + \frac{3\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{42} + \frac{3\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{21}$$

$$\boxed{\text{z39}} \quad \mathbb{Q}_5^{(c)}(A_{1u}) = \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{7}$$

$$\boxed{\text{z40}} \quad \mathbb{G}_0^{(c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z41}} \quad \mathbb{G}_2^{(c)}(A_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z42}} \quad \mathbb{G}_2^{(c)}(A_{1u}, b) = -\frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{5\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{84} + \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{5\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{84} - \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z43}} \quad \mathbb{G}_2^{(c)}(A_{1u}, c) = \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z44}} \quad \mathbb{G}_2^{(c)}(A_{1u}, d) = \frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z45}} \quad \mathbb{G}_4^{(c)}(A_{1u}, 1) = -\frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z63}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, a) = \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z64}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, b) = \mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z65}} \quad \mathbb{Q}_4^{(c)}(A_{2g}, c) = -\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z66}} \quad \mathbb{G}_1^{(c)}(A_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z67}} \quad \mathbb{G}_1^{(c)}(A_{2g}, b) = \frac{\sqrt{30}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{30}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{5}$$

$$\boxed{\text{z68}} \quad \mathbb{G}_3^{(c)}(A_{2g}, a) = -\frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z69}} \quad \mathbb{G}_3^{(c)}(A_{2g}, b) = -\frac{\sqrt{5}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{5} + \frac{\sqrt{5}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{5}$$

$$\boxed{\text{z70}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, a) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z89}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z90}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, c) = -\frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} - \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{21} - \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} - \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z91}} \quad \mathbb{Q}_1^{(c)}(A_{2u}, d) = -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z92}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, a) = \mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z93}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, b) = -\frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} - \frac{5\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{84} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{5\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{84} - \frac{4\sqrt{21}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z94}} \quad \mathbb{Q}_3^{(c)}(A_{2u}, c) = -\frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z95}} \quad \mathbb{Q}_5^{(c)}(A_{2u}, 2) = \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4}$$

$$\boxed{\text{z131}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z132}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, b) = \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z133}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, c) = \frac{3\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{42} - \frac{3\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{42} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{21}$$

$$\boxed{\text{z134}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, d) = -\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z135}} \quad \mathbb{Q}_2^{(c)}(B_{1g}, e) = -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z136}} \quad \mathbb{Q}_4^{(c)}(B_{1g}) = \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z137}} \quad \mathbb{G}_3^{(c)}(B_{1g}, a) = -\frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z138}} \quad \mathbb{G}_3^{(c)}(B_{1g}, b) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z139}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z140}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) = \mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z141}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, c) = -\frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z142}} \quad \mathbb{Q}_3^{(c)}(B_{1u}, d) = \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z143}} \quad \mathbb{Q}_5^{(c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z144}} \quad \mathbb{G}_2^{(c)}(B_{1u}, a) = \mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z145}} \quad \mathbb{G}_2^{(c)}(B_{1u}, b) = -\frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z146}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z147}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, b) = -\frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{7} + \frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{21} - \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{7} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{21} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{21}$$

$$\boxed{\text{z148}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, c) = -\frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z149}} \quad \mathbb{Q}_2^{(c)}(B_{2g}, d) = \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_3^{(b)}(B_{2u})$$

$$\boxed{\text{z150}} \quad \mathbb{Q}_4^{(c)}(B_{2g}) = -\frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{28} - \frac{3\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{28} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{28} - \frac{3\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{28} + \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z151}} \quad \mathbb{G}_3^{(c)}(B_{2g}, a) = \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{1,2}^{(b)}(E_u)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z152}} \quad \mathbb{G}_3^{(c)}(B_{2g}, b) = -\frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z153}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, a) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} - \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z154}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) = \mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z155}} \quad \mathbb{Q}_3^{(c)}(B_{2u}, c) = \frac{\sqrt{3}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} - \frac{\sqrt{5}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{5}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{3}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z156}} \quad \mathbb{Q}_5^{(c)}(B_{2u}) = -\frac{\sqrt{105}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{21} - \frac{\sqrt{7}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} + \frac{\sqrt{105}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} + \frac{\sqrt{7}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{105}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{21}$$

$$\boxed{\text{z157}} \quad \mathbb{G}_2^{(c)}(B_{2u}, a) = -\frac{\sqrt{6}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{3}$$

$$\boxed{\text{z158}} \quad \mathbb{G}_2^{(c)}(B_{2u}, b) = -\frac{3\sqrt{21}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{\sqrt{35}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{3\sqrt{21}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{35}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{21}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})}{7}$$

$$\boxed{\text{z159}} \quad \mathbb{G}_2^{(c)}(B_{2u}, c) = \mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z160}} \quad \mathbb{G}_2^{(c)}(B_{2u}, d) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z197}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z198}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z199}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z200}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z201}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, c) = -\frac{\sqrt{14}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{14} - \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{42} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{42} - \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{42}$$

$$\boxed{\text{z202}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, c) = -\frac{\sqrt{14}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{14} - \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{42} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{42} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{42}$$

$$\boxed{\text{z203}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, d) = -\frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} + \frac{\sqrt{30}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z226}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, d) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} - \frac{\sqrt{30}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z227}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, e) = \frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} + \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z228}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, e) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} - \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z229}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1a) = \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z230}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1a) = \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z231}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1b) = -\frac{\sqrt{30}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} - \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z232}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1b) = \frac{\sqrt{30}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_3^{(b)}(B_{2u})}{8} + \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_3^{(b)}(B_{2u})}{8}$$

$$\boxed{\text{z233}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 1c) = -\frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z250}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 1c) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_3^{(b)}(B_{2u})}{2}$$

$$\boxed{\text{z251}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g, 2) = -\frac{\sqrt{70}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{56} + \frac{3\sqrt{42}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{56} - \frac{\sqrt{70}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{56} + \frac{\sqrt{42}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{14} + \frac{3\sqrt{42}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{56}$$

$$\boxed{\text{z252}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g, 2) = -\frac{\sqrt{70}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{56} + \frac{3\sqrt{42}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{56} - \frac{\sqrt{70}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{56} + \frac{\sqrt{42}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{14} - \frac{3\sqrt{42}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{56}$$

$$\boxed{\text{z253}} \quad \mathbb{G}_{1,1}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z254}} \quad \mathbb{G}_{1,2}^{(c)}(E_g, a) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z255}} \quad \mathbb{G}_{1,1}^{(c)}(E_g, b) = -\frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z256}} \quad \mathbb{G}_{1,2}^{(c)}(E_g, b) = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z277}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 1a) = -\frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z278}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 1a) = -\frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8}$$

$$\boxed{\text{z279}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 1b) = \frac{\sqrt{10}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{30}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{20} - \frac{\sqrt{10}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z280}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 1b) = \frac{\sqrt{10}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{30}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{20} + \frac{\sqrt{10}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{10}$$

$$\boxed{\text{z281}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 2a) = \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{24} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{24}$$

$$\boxed{\text{z282}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 2a) = \frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_1^{(b)}(A_{2u})}{8} - \frac{\sqrt{6}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_1^{(b)}(A_{2u})}{24} + \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{8} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{24}$$

$$\boxed{\text{z283}} \quad \mathbb{G}_{3,1}^{(c)}(E_g, 2b) = \frac{\sqrt{6}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} - \frac{\sqrt{2}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z284}} \quad \mathbb{G}_{3,2}^{(c)}(E_g, 2b) = \frac{\sqrt{6}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_1^{(b)}(A_{2u})}{6} + \frac{\sqrt{2}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{1,2}^{(b)}(E_u)}{12} - \frac{\sqrt{6}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{1,1}^{(b)}(E_u)}{6}$$

$$\boxed{\text{z321}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z322}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z323}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, b) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z324}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, b) = -\frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z325}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, c) = \frac{3\sqrt{14}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{28} - \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{84} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{42}$$

$$\boxed{\text{z326}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, c) = -\frac{3\sqrt{14}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{28} + \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{84} - \frac{\sqrt{14}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} + \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{42} - \frac{\sqrt{210}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42}$$

$$\boxed{\text{z327}} \quad \mathbb{Q}_{1,1}^{(c)}(E_u, d) = \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{6} - \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z328}} \quad \mathbb{Q}_{1,2}^{(c)}(E_u, d) = -\frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{6} + \frac{\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{3}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z329}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1a) = \frac{\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z330}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1a) = -\frac{\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z331}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1b) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z332}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1b) = \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z333}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1c) = \frac{33\sqrt{1834}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{3668} + \frac{17\sqrt{27510}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{11004} - \frac{2\sqrt{1834}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{917} - \frac{17\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5502} + \frac{2\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2751}$$

$$\boxed{\text{z334}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1c) = -\frac{33\sqrt{1834}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{3668} - \frac{17\sqrt{27510}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{11004} - \frac{2\sqrt{1834}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{917} - \frac{17\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{5502} - \frac{2\sqrt{27510}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2751}$$

$$\boxed{\text{z335}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 1d) = -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{30} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{30} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z336}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 1d) = \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{30} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6}$$

$$\boxed{\text{z337}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2a) = \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

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

$$\boxed{\text{z339}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2b) = \frac{25\sqrt{655}\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} - \frac{5\sqrt{393}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} - \frac{7\sqrt{655}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{1048} + \frac{5\sqrt{393}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{1048} - \frac{4\sqrt{393}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{131}$$

$$\boxed{\text{z340}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2b) = -\frac{25\sqrt{655}\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} + \frac{5\sqrt{393}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} - \frac{7\sqrt{655}\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{1048} + \frac{5\sqrt{393}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{1048} + \frac{4\sqrt{393}\mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{131}$$

$$\boxed{\text{z341}} \quad \mathbb{Q}_{3,1}^{(c)}(E_u, 2c) = \frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{10} + \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z342}} \quad \mathbb{Q}_{3,2}^{(c)}(E_u, 2c) = -\frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{10} - \frac{\sqrt{5}\mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} - \frac{\sqrt{15}\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z343}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 1) = \frac{5\mathbb{Q}_{3,1}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{16} - \frac{\sqrt{15}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{80} + \frac{5\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{8} + \frac{\sqrt{15}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{40}$$

$$\boxed{\text{z344}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 1) = -\frac{5\mathbb{Q}_{3,2}^{(a)}(E_u, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{16} + \frac{\sqrt{15}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{80} + \frac{5\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{8} + \frac{\sqrt{15}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{40}$$

$$\boxed{\text{z345}} \quad \mathbb{Q}_{5,1}^{(c)}(E_u, 2) = -\frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{5} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z346}} \quad \mathbb{Q}_{5,2}^{(c)}(E_u, 2) = \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(E_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})}{5} - \frac{\sqrt{10}\mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}$$

$$\boxed{\text{z347}} \quad \mathbb{G}_{2,1}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z348}} \quad \mathbb{G}_{2,2}^{(c)}(E_u, a) = \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z349}} \quad \mathbb{G}_{2,1}^{(c)}(E_u, b) = -\frac{\mathbb{G}_{2,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z350}} \quad \mathbb{G}_{2,2}^{(c)}(E_u, b) = \frac{\mathbb{G}_{2,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

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

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

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

$$\boxed{x3} \quad \mathbb{Q}_4^{(a)}(A_{1g}, 1) = \begin{bmatrix} \frac{\sqrt{30}}{10} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{30}}{10} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{30}}{15} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{15} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{30}}{15} \end{bmatrix}$$

$$\boxed{x4} \quad \mathbb{Q}_4^{(a)}(A_{1g}, 2) = \begin{bmatrix} \frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{21} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}}{21} & 0 \\ 0 & 0 & 0 & 0 & \frac{2\sqrt{42}}{21} \end{bmatrix}$$

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

$$\boxed{x6} \quad \mathbb{Q}_2^{(a)}(B_{1g}) = \begin{bmatrix} 0 & -\frac{\sqrt{14}}{7} & 0 & 0 & 0 \\ -\frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}}{14} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x7} \quad \mathbb{Q}_4^{(a)}(B_{1g}) = \begin{bmatrix} 0 & -\frac{\sqrt{42}}{14} & 0 & 0 & 0 \\ -\frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{14}}{7} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x8} \quad \mathbb{Q}_2^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{\sqrt{14}}{7} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{42}}{14} & 0 \\ 0 & 0 & \frac{\sqrt{42}}{14} & 0 & 0 \\ -\frac{\sqrt{14}}{7} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x9} \quad \mathbb{Q}_4^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{14} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{14}}{7} & 0 \\ 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0 \\ \frac{\sqrt{42}}{14} & 0 & 0 & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{x12} \quad \mathbb{Q}_{4,1}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}}{4} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{6}}{4} & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x13} \quad \mathbb{Q}_{4,2}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{6}}{4} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{6}}{4} & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x14} \quad \mathbb{Q}_{4,1}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{42}}{28} & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{14}}{28} & 0 & 0 \\ -\frac{\sqrt{42}}{28} & \frac{3\sqrt{14}}{28} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{7} \\ 0 & 0 & 0 & \frac{\sqrt{14}}{7} & 0 \end{bmatrix}$$

$$\boxed{x15} \quad \mathbb{Q}_{4,2}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{42}}{28} & 0 \\ 0 & 0 & 0 & -\frac{3\sqrt{14}}{28} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{14}}{7} \\ -\frac{\sqrt{42}}{28} & -\frac{3\sqrt{14}}{28} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{14}}{7} & 0 & 0 \end{bmatrix}$$

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

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

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

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

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

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

$$\boxed{x22} \quad \mathbb{M}_{3,1}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{30}i}{20} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{20} & 0 & 0 \\ \frac{\sqrt{30}i}{20} & \frac{\sqrt{10}i}{20} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{10}i}{5} \\ 0 & 0 & 0 & -\frac{\sqrt{10}i}{5} & 0 \end{bmatrix}$$

$$\boxed{x23} \quad \mathbb{M}_{3,2}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{30}i}{20} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{10}i}{20} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{10}i}{5} \\ \frac{\sqrt{30}i}{20} & -\frac{\sqrt{10}i}{20} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{5} & 0 & 0 \end{bmatrix}$$

$$\boxed{x24} \quad \mathbb{M}_{3,1}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{4} & 0 & 0 \\ \frac{\sqrt{2}i}{4} & -\frac{\sqrt{6}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x25} \quad \mathbb{M}_{3,2}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{2}i}{4} & \frac{\sqrt{6}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

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

$$\boxed{x26} \quad \mathbb{Q}_0^{(a)}(A_{1g}) = \begin{bmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$$

$$\boxed{x27} \quad \mathbb{Q}_2^{(a)}(A_{1g}) = \begin{bmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{bmatrix}$$

$$\boxed{x28} \quad \mathbb{Q}_2^{(a)}(B_{1g}) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x29} \quad \mathbb{Q}_2^{(a)}(B_{2g}) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{x32} \quad \mathbb{M}_1^{(a)}(A_{2g}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

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

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

- bra: $\langle f_3 |, \langle f_{ax} |, \langle f_{ay} |, \langle f_{az} |, \langle f_{bx} |, \langle f_{by} |, \langle f_{bz} |$
- ket: $|f_3\rangle, |f_{ax}\rangle, |f_{ay}\rangle, |f_{az}\rangle, |f_{bx}\rangle, |f_{by}\rangle, |f_{bz}\rangle$

$$\boxed{x35} \quad \mathbb{Q}_0^{(a)}(A_{1g}) = \begin{bmatrix} \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{7} \end{bmatrix}$$

$$\boxed{x36} \quad \mathbb{Q}_2^{(a)}(A_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{21}}{21} & 0 & 0 & \frac{\sqrt{35}}{14} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{21}}{21} & 0 & 0 & -\frac{\sqrt{35}}{14} & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{21}}{21} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{35}}{14} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{35}}{14} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x37} \quad \mathbb{Q}_4^{(a)}(A_{1g}, 1) = \begin{bmatrix} -\frac{\sqrt{66}}{11} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{66} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{66} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{66} \end{bmatrix}$$

$$\boxed{x38} \quad \mathbb{Q}_4^{(a)}(A_{1g}, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2310}}{308} & 0 & 0 & -\frac{3\sqrt{154}}{308} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2310}}{308} & 0 & 0 & \frac{3\sqrt{154}}{308} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{2310}}{154} & 0 & 0 & 0 \\ 0 & -\frac{3\sqrt{154}}{308} & 0 & 0 & \frac{\sqrt{2310}}{132} & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{154}}{308} & 0 & 0 & \frac{\sqrt{2310}}{132} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2310}}{66} \end{bmatrix}$$

$$\boxed{x39} \quad \mathbb{Q}_6^{(a)}(A_{1g}, 1) = \begin{bmatrix} \frac{2\sqrt{462}}{77} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{5\sqrt{462}}{462} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{5\sqrt{462}}{462} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{5\sqrt{462}}{462} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{3\sqrt{462}}{154} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{3\sqrt{462}}{154} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3\sqrt{462}}{154} \end{bmatrix}$$

$$\boxed{x40} \quad \mathbb{Q}_6^{(a)}(A_{1g}, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{5\sqrt{66}}{132} & 0 & 0 & -\frac{\sqrt{110}}{44} & 0 & 0 \\ 0 & 0 & -\frac{5\sqrt{66}}{132} & 0 & 0 & \frac{\sqrt{110}}{44} & 0 \\ 0 & 0 & 0 & \frac{5\sqrt{66}}{66} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{110}}{44} & 0 & 0 & -\frac{\sqrt{66}}{44} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{110}}{44} & 0 & 0 & -\frac{\sqrt{66}}{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{66}}{22} \end{bmatrix}$$

$$\boxed{x41} \quad \mathbb{Q}_4^{(a)}(A_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{110}}{22} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{22} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{22} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{110}}{22} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x42} \quad \mathbb{Q}_6^{(a)}(A_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{33}}{11} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{55}}{22} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{55}}{22} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{55}}{22} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{55}}{22} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{33}}{11} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x43} \quad \mathbb{Q}_2^{(a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{7}}{7} & 0 & 0 & \frac{\sqrt{105}}{42} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{7}}{7} & 0 & 0 & \frac{\sqrt{105}}{42} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{105}}{21} \\ 0 & \frac{\sqrt{105}}{42} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{105}}{42} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{105}}{21} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x44} \quad \mathbb{Q}_4^{(a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3\sqrt{770}}{308} & 0 & 0 & -\frac{\sqrt{462}}{308} & 0 & 0 \\ 0 & 0 & -\frac{3\sqrt{770}}{308} & 0 & 0 & -\frac{\sqrt{462}}{308} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{462}}{154} \\ 0 & -\frac{\sqrt{462}}{308} & 0 & 0 & -\frac{\sqrt{770}}{44} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{462}}{308} & 0 & 0 & \frac{\sqrt{770}}{44} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{462}}{154} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x45} \quad \mathbb{Q}_6^{(a)}(B_{1g}, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x46} \quad \mathbb{Q}_6^{(a)}(B_{1g}, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{5\sqrt{22}}{44} & 0 & 0 & -\frac{\sqrt{330}}{132} & 0 & 0 \\ 0 & 0 & -\frac{5\sqrt{22}}{44} & 0 & 0 & -\frac{\sqrt{330}}{132} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{330}}{66} \\ 0 & -\frac{\sqrt{330}}{132} & 0 & 0 & \frac{3\sqrt{22}}{44} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{330}}{132} & 0 & 0 & -\frac{3\sqrt{22}}{44} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{330}}{66} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x47} \quad \mathbb{Q}_2^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{105}}{21} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & -\frac{\sqrt{105}}{84} & 0 \\ 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & \frac{\sqrt{105}}{84} & 0 & 0 \\ -\frac{\sqrt{105}}{21} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{105}}{84} & 0 & 0 & -\frac{5\sqrt{7}}{28} & 0 \\ 0 & -\frac{\sqrt{105}}{84} & 0 & 0 & -\frac{5\sqrt{7}}{28} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x48} \quad \mathbb{Q}_4^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{462}}{154} & 0 & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{770}}{154} & 0 & 0 & -\frac{\sqrt{462}}{77} & 0 \\ 0 & \frac{3\sqrt{770}}{154} & 0 & 0 & \frac{\sqrt{462}}{77} & 0 & 0 \\ -\frac{\sqrt{462}}{154} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{462}}{77} & 0 & 0 & \frac{\sqrt{770}}{154} & 0 \\ 0 & -\frac{\sqrt{462}}{77} & 0 & 0 & \frac{\sqrt{770}}{154} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x49} \quad \mathbb{Q}_6^{(a)}(B_{2g}, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{5\sqrt{2}}{16} & 0 & 0 & -\frac{\sqrt{30}}{16} & 0 \\ 0 & -\frac{5\sqrt{2}}{16} & 0 & 0 & \frac{\sqrt{30}}{16} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{30}}{16} & 0 & 0 & \frac{3\sqrt{2}}{16} & 0 \\ 0 & -\frac{\sqrt{30}}{16} & 0 & 0 & \frac{3\sqrt{2}}{16} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x50} \quad \mathbb{Q}_6^{(a)}(B_{2g}, 2) = \begin{bmatrix} 0 & 0 & 0 & \frac{2\sqrt{66}}{33} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{110}}{176} & 0 & 0 & -\frac{13\sqrt{66}}{528} & 0 \\ 0 & \frac{\sqrt{110}}{176} & 0 & 0 & \frac{13\sqrt{66}}{528} & 0 & 0 \\ \frac{2\sqrt{66}}{33} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{13\sqrt{66}}{528} & 0 & 0 & -\frac{7\sqrt{110}}{176} & 0 \\ 0 & -\frac{13\sqrt{66}}{528} & 0 & 0 & -\frac{7\sqrt{110}}{176} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x51} \quad \mathbb{Q}_{2,1}^{(a)}(E_g) = \begin{bmatrix} 0 & -\frac{\sqrt{105}}{21} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{105}}{21} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & -\frac{\sqrt{105}}{84} \\ 0 & 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & \frac{\sqrt{105}}{84} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{105}}{84} & 0 & 0 & -\frac{5\sqrt{7}}{28} \\ 0 & 0 & -\frac{\sqrt{105}}{84} & 0 & 0 & -\frac{5\sqrt{7}}{28} & 0 \end{bmatrix}$$

$$\boxed{x52} \quad \mathbb{Q}_{2,2}^{(a)}(E_g) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{105}}{21} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & \frac{\sqrt{105}}{84} \\ -\frac{\sqrt{105}}{21} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{7}}{28} & 0 & 0 & -\frac{\sqrt{105}}{84} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{105}}{84} & 0 & 0 & -\frac{5\sqrt{7}}{28} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{105}}{84} & 0 & 0 & -\frac{5\sqrt{7}}{28} & 0 & 0 \end{bmatrix}$$

$$\boxed{x53} \quad \mathbb{Q}_{4,1}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{110}}{22} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{22} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{22} & 0 \\ \frac{\sqrt{110}}{22} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{66}}{22} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x54} \quad \mathbb{Q}_{4,2}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{110}}{22} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{66}}{22} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{66}}{22} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 \\ -\frac{\sqrt{110}}{22} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x55} \quad \mathbb{Q}_{4,1}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & -\frac{\sqrt{462}}{154} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{462}}{154} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{770}}{154} & 0 & 0 & -\frac{\sqrt{462}}{77} \\ 0 & 0 & \frac{3\sqrt{770}}{154} & 0 & 0 & \frac{\sqrt{462}}{77} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{462}}{77} & 0 & 0 & \frac{\sqrt{770}}{154} \\ 0 & 0 & -\frac{\sqrt{462}}{77} & 0 & 0 & \frac{\sqrt{770}}{154} & 0 \end{bmatrix}$$

$$\boxed{x56} \quad \mathbb{Q}_{4,2}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{462}}{154} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{770}}{154} & 0 & 0 & \frac{\sqrt{462}}{77} \\ -\frac{\sqrt{462}}{154} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3\sqrt{770}}{154} & 0 & 0 & -\frac{\sqrt{462}}{77} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{462}}{77} & 0 & 0 & \frac{\sqrt{770}}{154} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{462}}{77} & 0 & 0 & \frac{\sqrt{770}}{154} & 0 & 0 \end{bmatrix}$$

$$\boxed{x57} \quad \mathbb{Q}_{6,1}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{33}}{11} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{55}}{22} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{55}}{22} & 0 \\ \frac{\sqrt{33}}{11} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{55}}{22} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{55}}{22} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x58} \quad \mathbb{Q}_{6,2}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{33}}{11} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{55}}{22} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{55}}{22} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{55}}{22} & 0 & 0 & 0 \\ -\frac{\sqrt{33}}{11} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{55}}{22} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x59} \quad \mathbb{Q}_{6,1}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{5\sqrt{2}}{16} & 0 & 0 & -\frac{\sqrt{30}}{16} \\ 0 & 0 & -\frac{5\sqrt{2}}{16} & 0 & 0 & \frac{\sqrt{30}}{16} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{30}}{16} & 0 & 0 & \frac{3\sqrt{2}}{16} \\ 0 & 0 & -\frac{\sqrt{30}}{16} & 0 & 0 & \frac{3\sqrt{2}}{16} & 0 \end{bmatrix}$$

$$\boxed{x60} \quad \mathbb{Q}_{6,2}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{5\sqrt{2}}{16} & 0 & 0 & \frac{\sqrt{30}}{16} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{5\sqrt{2}}{16} & 0 & 0 & -\frac{\sqrt{30}}{16} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{16} & 0 & 0 & \frac{3\sqrt{2}}{16} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{30}}{16} & 0 & 0 & \frac{3\sqrt{2}}{16} & 0 & 0 \end{bmatrix}$$

$$\boxed{x61} \quad \mathbb{Q}_{6,1}^{(a)}(E_g, 3) = \begin{bmatrix} 0 & \frac{2\sqrt{66}}{33} & 0 & 0 & 0 & 0 & 0 \\ \frac{2\sqrt{66}}{33} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{110}}{176} & 0 & 0 & -\frac{13\sqrt{66}}{528} \\ 0 & 0 & \frac{\sqrt{110}}{176} & 0 & 0 & \frac{13\sqrt{66}}{528} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{13\sqrt{66}}{528} & 0 & 0 & -\frac{7\sqrt{110}}{176} \\ 0 & 0 & -\frac{13\sqrt{66}}{528} & 0 & 0 & -\frac{7\sqrt{110}}{176} & 0 \end{bmatrix}$$

$$\boxed{x62} \quad \mathbb{Q}_{6,2}^{(a)}(E_g, 3) = \begin{bmatrix} 0 & 0 & \frac{2\sqrt{66}}{33} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{110}}{176} & 0 & 0 & \frac{13\sqrt{66}}{528} \\ \frac{2\sqrt{66}}{33} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{110}}{176} & 0 & 0 & -\frac{13\sqrt{66}}{528} & 0 & 0 \\ 0 & 0 & 0 & -\frac{13\sqrt{66}}{528} & 0 & 0 & -\frac{7\sqrt{110}}{176} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{13\sqrt{66}}{528} & 0 & 0 & -\frac{7\sqrt{110}}{176} & 0 & 0 \end{bmatrix}$$

$$\boxed{x63} \quad \mathbb{M}_5^{(a)}(A_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x64} \quad \mathbb{M}_1^{(a)}(A_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{7} \\ 0 & 0 & \frac{3\sqrt{7}i}{28} & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 \\ 0 & -\frac{3\sqrt{7}i}{28} & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 & -\frac{\sqrt{7}i}{28} & 0 \\ 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 & \frac{\sqrt{7}i}{28} & 0 & 0 \\ -\frac{\sqrt{7}i}{7} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x65} \quad \mathbb{M}_3^{(a)}(A_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x66} \quad \mathbb{M}_5^{(a)}(A_{2g}, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\frac{2\sqrt{21}i}{21} \\ 0 & 0 & -\frac{5\sqrt{21}i}{168} & 0 & 0 & \frac{3\sqrt{35}i}{56} & 0 \\ 0 & \frac{5\sqrt{21}i}{168} & 0 & 0 & \frac{3\sqrt{35}i}{56} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{3\sqrt{35}i}{56} & 0 & 0 & \frac{11\sqrt{21}i}{168} & 0 \\ 0 & -\frac{3\sqrt{35}i}{56} & 0 & 0 & -\frac{11\sqrt{21}i}{168} & 0 & 0 \\ \frac{2\sqrt{21}i}{21} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x67} \quad \mathbb{M}_5^{(a)}(A_{2g}, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{8} & 0 & 0 & -\frac{i}{8} & 0 \\ 0 & -\frac{\sqrt{15}i}{8} & 0 & 0 & -\frac{i}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{i}{8} & 0 & 0 & \frac{\sqrt{15}i}{8} & 0 \\ 0 & \frac{i}{8} & 0 & 0 & -\frac{\sqrt{15}i}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x68} \quad \mathbb{M}_3^{(a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x69} \quad \mathbb{M}_5^{(a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{3} \\ 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}i}{3} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x70} \quad \mathbb{M}_3^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x71} \quad \mathbb{M}_5^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{3}i}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x72} \quad \mathbb{M}_{1,1}^{(a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{7} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{7}i}{28} & 0 & 0 & \frac{\sqrt{105}i}{28} \\ 0 & 0 & -\frac{3\sqrt{7}i}{28} & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 \\ -\frac{\sqrt{7}i}{7} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 & -\frac{\sqrt{7}i}{28} \\ 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 & \frac{\sqrt{7}i}{28} & 0 \end{bmatrix}$$

$$\boxed{x73} \quad \mathbb{M}_{1,2}^{(a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{7}i}{7} & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{7}i}{28} & 0 & 0 & -\frac{\sqrt{105}i}{28} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{3\sqrt{7}i}{28} & 0 & 0 & -\frac{\sqrt{105}i}{28} & 0 & 0 \\ \frac{\sqrt{7}i}{7} & 0 & 0 & \frac{\sqrt{105}i}{28} & 0 & 0 & -\frac{\sqrt{7}i}{28} \\ 0 & \frac{\sqrt{105}i}{28} & 0 & 0 & \frac{\sqrt{7}i}{28} & 0 & 0 \end{bmatrix}$$

$$\boxed{x74} \quad \mathbb{M}_{3,1}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$$

$$\boxed{x75} \quad \mathbb{M}_{3,2}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \end{bmatrix}$$

$$\boxed{x76} \quad \mathbb{M}_{3,1}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x77} \quad \mathbb{M}_{3,2}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x78} \quad \mathbb{M}_{5,1}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{2\sqrt{21}i}{21} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{5\sqrt{21}i}{168} & 0 & 0 & \frac{3\sqrt{35}i}{56} \\ 0 & 0 & \frac{5\sqrt{21}i}{168} & 0 & 0 & \frac{3\sqrt{35}i}{56} & 0 \\ \frac{2\sqrt{21}i}{21} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{3\sqrt{35}i}{56} & 0 & 0 & \frac{11\sqrt{21}i}{168} \\ 0 & 0 & -\frac{3\sqrt{35}i}{56} & 0 & 0 & -\frac{11\sqrt{21}i}{168} & 0 \end{bmatrix}$$

$$\boxed{x79} \quad \mathbb{M}_{5,2}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{21}i}{21} & 0 \\ 0 & 0 & 0 & -\frac{5\sqrt{21}i}{168} & 0 & 0 & -\frac{3\sqrt{35}i}{56} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{5\sqrt{21}i}{168} & 0 & 0 & -\frac{3\sqrt{35}i}{56} & 0 & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{35}i}{56} & 0 & 0 & \frac{11\sqrt{21}i}{168} \\ -\frac{2\sqrt{21}i}{21} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3\sqrt{35}i}{56} & 0 & 0 & -\frac{11\sqrt{21}i}{168} & 0 & 0 \end{bmatrix}$$

$$\boxed{x80} \quad \mathbb{M}_{5,1}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}i}{8} & 0 & 0 & -\frac{i}{8} \\ 0 & 0 & -\frac{\sqrt{15}i}{8} & 0 & 0 & -\frac{i}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{8} & 0 & 0 & \frac{\sqrt{15}i}{8} \\ 0 & 0 & \frac{i}{8} & 0 & 0 & -\frac{\sqrt{15}i}{8} & 0 \end{bmatrix}$$

$$\boxed{x81} \quad \mathbb{M}_{5,2}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}i}{8} & 0 & 0 & \frac{i}{8} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{15}i}{8} & 0 & 0 & \frac{i}{8} & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{8} & 0 & 0 & \frac{\sqrt{15}i}{8} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{i}{8} & 0 & 0 & -\frac{\sqrt{15}i}{8} & 0 & 0 \end{bmatrix}$$

$$\boxed{x82} \quad \mathbb{M}_{5,1}^{(a)}(E_g, 3) = \begin{bmatrix} 0 & -\frac{\sqrt{3}i}{3} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{3}i}{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x83} \quad \mathbb{M}_{5,2}^{(a)}(E_g, 3) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{3}i}{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}i}{6} \\ \frac{\sqrt{3}i}{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Cluster SAMB

- Site cluster

** Wyckoff: 2a

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

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

** Wyckoff: 2c

$$\boxed{y3} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2} \right]$$

$$\boxed{y4} \quad \mathbb{Q}_1^{(s)}(A_{2u}) = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

** Wyckoff: 2b

$$\boxed{y5} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2} \right]$$

$$\boxed{y6} \quad \mathbb{Q}_3^{(s)}(B_{2u}) = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

- Bond cluster

** Wyckoff: 8a@8i

$$\boxed{y7} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4} \right]$$

$$\boxed{y8} \quad \mathbb{T}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4} \right]$$

$$\boxed{y9} \quad \mathbb{Q}_1^{(s)}(A_{2u}) = \left[\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4} \right]$$

$$\boxed{y10} \quad \mathbb{T}_1^{(s)}(A_{2u}) = \left[\frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4} \right]$$

$$\boxed{y11} \quad \mathbb{Q}_2^{(s)}(B_{1g}) = \left[\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4} \right]$$

$$\boxed{y12} \quad \mathbb{T}_2^{(s)}(B_{1g}) = \left[\frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4} \right]$$

$$\boxed{y13} \quad \mathbb{M}_2^{(s)}(B_{2u}) = \left[\frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, -\frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4}, \frac{\sqrt{2}i}{4} \right]$$

$$\boxed{y14} \quad \mathbb{Q}_3^{(s)}(B_{2u}) = \left[\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, -\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4} \right]$$

$$\boxed{y15} \quad \mathbb{Q}_{2,1}^{(s)}(E_g) = \left[\frac{1}{2}, -\frac{1}{2}, 0, 0, -\frac{1}{2}, \frac{1}{2}, 0, 0 \right]$$

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

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

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

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

$$\boxed{y20} \quad \mathbb{Q}_{1,2}^{(s)}(E_u) = \left[\frac{1}{2}, -\frac{1}{2}, 0, 0, \frac{1}{2}, -\frac{1}{2}, 0, 0 \right]$$

$$\boxed{y21} \quad \mathbb{T}_{1,1}^{(s)}(E_u) = \left[0, 0, -\frac{i}{2}, \frac{i}{2}, 0, 0, \frac{i}{2}, -\frac{i}{2} \right]$$

$$\boxed{y22} \quad \mathbb{T}_{1,2}^{(s)}(E_u) = \left[\frac{i}{2}, -\frac{i}{2}, 0, 0, \frac{i}{2}, -\frac{i}{2}, 0, 0 \right]$$

Table 5: Orbital of each site

| # | site | orbital |
|---|------|---|
| 1 | Pt1 | $ d_u\rangle, d_v\rangle, d_{yz}\rangle, d_{xz}\rangle, d_{xy}\rangle$ |
| 2 | Pt2 | $ d_u\rangle, d_v\rangle, d_{yz}\rangle, d_{xz}\rangle, d_{xy}\rangle$ |
| 3 | Si1 | $ p_x\rangle, p_y\rangle, p_z\rangle$ |
| 4 | Si2 | $ p_x\rangle, p_y\rangle, p_z\rangle$ |
| 5 | U | $ f_3\rangle, f_{ax}\rangle, f_{ay}\rangle, f_{az}\rangle, f_{bx}\rangle, f_{by}\rangle, f_{bz}\rangle$ |

Table 6: Neighbor and bra-ket of each bond

| # | head | tail | neighbor | head (bra) | tail (ket) |
|---|------|------|----------|------------|------------|
| 1 | Pt1 | Si2 | [1] | [d] | [p] |
| 2 | Pt2 | Si1 | [1] | [d] | [p] |

— Site in Unit Cell —

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

Table 7: 'Pt1' (#1) site cluster (2a), -4m2

| SL | position (s) | mapping |
|----|------------------------------|-----------------------|
| 1 | [0.75000, 0.25000, 0.00000] | [1,2,7,8,11,12,13,14] |
| 2 | [0.25000, 0.75000, 0.00000] | [3,4,5,6,9,10,15,16] |

Table 8: 'Pt2' (#2) site cluster (2c), 4mm

| SL | position (s) | mapping |
|----|------------------------------|-----------------------|
| 1 | [0.25000, 0.25000, 0.37850] | [1,2,3,4,13,14,15,16] |
| 2 | [0.75000, 0.75000, 0.62150] | [5,6,7,8,9,10,11,12] |

Table 9: 'Si1' (#3) site cluster (2b), -4m2

| SL | position (s) | mapping |
|----|------------------------------|-----------------------|
| 1 | [0.75000, 0.25000, 0.50000] | [1,2,7,8,11,12,13,14] |
| 2 | [0.25000, 0.75000, 0.50000] | [3,4,5,6,9,10,15,16] |

Table 10: 'Si2' (#4) site cluster (2c), 4mm

| SL | position (s) | mapping |
|----|------------------------------|-----------------------|
| 1 | [0.25000, 0.25000, 0.13300] | [1,2,3,4,13,14,15,16] |
| 2 | [0.75000, 0.75000, 0.86700] | [5,6,7,8,9,10,11,12] |

Table 11: 'U' (#5) site cluster (2c), 4mm

| SL | position (s) | mapping |
|----|------------------------------|-----------------------|
| 1 | [0.25000, 0.25000, 0.74840] | [1,2,3,4,13,14,15,16] |
| 2 | [0.75000, 0.75000, 0.25160] | [5,6,7,8,9,10,11,12] |

— Bond in Unit Cell —————

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

Table 12: 1-th 'Pt1'-'Si2' [1] (#1) bond cluster (8a@8i), D, $|\mathbf{v}| = 2.46277$ (cartesian)

| SL | vector (\mathbf{v}) | center (\mathbf{c}) | mapping | head | tail | \mathbf{R} (primitive) |
|----|--------------------------------|------------------------------|---------|-------|-------|--------------------------|
| 1 | [0.00000, 0.50000, -0.13300] | [0.25000, 0.50000, 0.06650] | [1,14] | (2,1) | (1,1) | [0,0,0] |
| 2 | [0.00000, -0.50000, -0.13300] | [0.25000, 0.00000, 0.06650] | [2,13] | (2,1) | (1,1) | [0,1,0] |
| 3 | [-0.50000, 0.00000, -0.13300] | [0.00000, 0.25000, 0.06650] | [3,15] | (1,1) | (1,1) | [1,0,0] |
| 4 | [0.50000, 0.00000, -0.13300] | [0.50000, 0.25000, 0.06650] | [4,16] | (1,1) | (1,1) | [0,0,0] |
| 5 | [0.00000, 0.50000, 0.13300] | [0.75000, 0.00000, 0.93350] | [5,10] | (1,1) | (2,1) | [0,-1,-1] |
| 6 | [0.00000, -0.50000, 0.13300] | [0.75000, 0.50000, 0.93350] | [6,9] | (1,1) | (2,1) | [0,0,-1] |
| 7 | [0.50000, 0.00000, 0.13300] | [0.00000, 0.75000, 0.93350] | [7,11] | (2,1) | (2,1) | [-1,0,-1] |
| 8 | [-0.50000, 0.00000, 0.13300] | [0.50000, 0.75000, 0.93350] | [8,12] | (2,1) | (2,1) | [0,0,-1] |

Table 13: 1-th 'Pt2'-'Si1' [1] (#2) bond cluster (8a@8i), D, $|\mathbf{v}| = 2.40633$ (cartesian)

| SL | vector (\mathbf{v}) | center (\mathbf{c}) | mapping | head | tail | \mathbf{R} (primitive) |
|----|--------------------------------|------------------------------|---------|-------|-------|--------------------------|
| 1 | [0.00000, 0.50000, -0.12150] | [0.25000, 0.00000, 0.43925] | [1,14] | (1,1) | (2,1) | [0,-1,0] |
| 2 | [0.00000, -0.50000, -0.12150] | [0.25000, 0.50000, 0.43925] | [2,13] | (1,1) | (2,1) | [0,0,0] |
| 3 | [-0.50000, 0.00000, -0.12150] | [0.50000, 0.25000, 0.43925] | [3,15] | (1,1) | (1,1) | [0,0,0] |
| 4 | [0.50000, 0.00000, -0.12150] | [0.00000, 0.25000, 0.43925] | [4,16] | (1,1) | (1,1) | [-1,0,0] |
| 5 | [0.00000, 0.50000, 0.12150] | [0.75000, 0.50000, 0.56075] | [5,10] | (2,1) | (1,1) | [0,0,0] |

continued ...

Table 13

| SL | vector (v) | center (c) | mapping | head | tail | R (primitive) |
|----|-------------------------------|------------------------------|---------|-------|-------|-----------------|
| 6 | [0.00000, -0.50000, 0.12150] | [0.75000, 0.00000, 0.56075] | [6,9] | (2,1) | (1,1) | [0,1,0] |
| 7 | [0.50000, 0.00000, 0.12150] | [0.50000, 0.75000, 0.56075] | [7,11] | (2,1) | (2,1) | [0,0,0] |
| 8 | [-0.50000, 0.00000, 0.12150] | [0.00000, 0.75000, 0.56075] | [8,12] | (2,1) | (2,1) | [1,0,0] |