

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 | $\{2_{001} \frac{1}{2}\frac{1}{2}0\}$ | 3 | $\{4_{001}^+ \frac{1}{2}00\}$ | 4 | $\{4_{001}^- 0\frac{1}{2}0\}$ | 5 | $\{2_{010} 0\frac{1}{2}0\}$ |
| 6 | $\{2_{100} \frac{1}{2}00\}$ | 7 | $\{2_{110} \frac{1}{2}\frac{1}{2}0\}$ | 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 | $Q_0(A_{1g})$ | A_{1g} | 0 | Q, T | - | - | 1 |
| 2 | $Q_2(A_{1g})$ | A_{1g} | 2 | Q, T | - | - | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| 3 | $Q_4(A_{1g}, 1)$ | 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 | $Q_4(A_{1g}, 2)$ | 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 | $G_5(A_{1g})$ | A_{1g} | 5 | G, M | - | - | $\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$ |
| 6 | $Q_6(A_{1g}, 1)$ | A_{1g} | 6 | Q, T | 1 | - | $\frac{\sqrt{2}(2x^6 - 15x^4y^2 - 15x^4z^2 - 15x^2y^4 + 180x^2y^2z^2 - 15x^2z^4 + 2y^6 - 15y^4z^2 - 15y^2z^4 + 2z^6)}{8}$ |
| 7 | $Q_6(A_{1g}, 2)$ | A_{1g} | 6 | Q, T | 2 | - | $-\frac{\sqrt{14}(x^6 - 15x^4z^2 + 15x^2z^4 + y^6 - 15y^4z^2 + 15y^2z^4 - 2z^6)}{8}$ |

continued ...

Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|----|---------------------------|----------|------|--------|--------------|-----------|---|
| 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 | - | $\frac{\sqrt{42}(x-y)(x+y)(x^4 - 9x^2y^2 - 5x^2z^2 + y^4 - 5y^2z^2 + 5z^4)}{8}$ |
| 28 | $\mathbb{G}_2(B_{1u})$ | B_{1u} | 2 | G, M | - | - | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |

continued ...

Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|----|----------------------------|----------|------|--------|--------------|-----------|--|
| 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 | $\frac{\sqrt{15}x(y-z)(y+z)}{2}$ |
| 49 | $\mathbb{G}_{3,2}(E_g, 2)$ | | | | | 2 | $-\frac{\sqrt{15}y(x-z)(x+z)}{2}$ |

continued ...

Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|----|----------------------------|--------|------|--------|--------------|-----------|--|
| 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 | $-\sqrt{3}xz$ |
| 70 | $\mathbb{Q}_{3,1}(E_u, 1)$ | E_u | 3 | Q, T | 1 | 1 | $\frac{x(2x^2-3y^2-3z^2)}{2}$ |

continued ...

Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|----|----------------------------|--------|------|--------|--------------|-----------|--|
| 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_v\rangle @Pt1(1)$ | 1 | $ d_{xy}\rangle @Pt1(1)$ | 2 | $ d_{xz}\rangle @Pt1(1)$ | 3 | $ d_{yz}\rangle @Pt1(1)$ | 4 | $ d_u\rangle @Pt1(1)$ |
| 5 | $ d_v\rangle @Pt1(2)$ | 6 | $ d_{xy}\rangle @Pt1(2)$ | 7 | $ d_{xz}\rangle @Pt1(2)$ | 8 | $ d_{yz}\rangle @Pt1(2)$ | 9 | $ d_u\rangle @Pt1(2)$ |
| 10 | $ d_v\rangle @Pt2(1)$ | 11 | $ d_{xy}\rangle @Pt2(1)$ | 12 | $ d_{xz}\rangle @Pt2(1)$ | 13 | $ d_{yz}\rangle @Pt2(1)$ | 14 | $ d_u\rangle @Pt2(1)$ |
| 15 | $ d_v\rangle @Pt2(2)$ | 16 | $ d_{xy}\rangle @Pt2(2)$ | 17 | $ d_{xz}\rangle @Pt2(2)$ | 18 | $ d_{yz}\rangle @Pt2(2)$ | 19 | $ d_u\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)$ |

continued ...

Table 3

| # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) |
|----|-------------------------------|----|-------------------------------|----|-------------------------------|----|-------------------------------|----|-------------------------------|
| 25 | $ p_z\rangle @\text{Si1}(2)$ | 26 | $ p_x\rangle @\text{Si2}(1)$ | 27 | $ p_y\rangle @\text{Si2}(1)$ | 28 | $ p_z\rangle @\text{Si2}(1)$ | 29 | $ p_x\rangle @\text{Si2}(2)$ |
| 30 | $ p_y\rangle @\text{Si2}(2)$ | 31 | $ p_z\rangle @\text{Si2}(2)$ | 32 | $ f_2\rangle @\text{U}(1)$ | 33 | $ f_1\rangle @\text{U}(1)$ | 34 | $ f_{bz}\rangle @\text{U}(1)$ |
| 35 | $ f_3\rangle @\text{U}(1)$ | 36 | $ f_{3x}\rangle @\text{U}(1)$ | 37 | $ f_{3y}\rangle @\text{U}(1)$ | 38 | $ f_{az}\rangle @\text{U}(1)$ | 39 | $ f_2\rangle @\text{U}(2)$ |
| 40 | $ f_1\rangle @\text{U}(2)$ | 41 | $ f_{bz}\rangle @\text{U}(2)$ | 42 | $ f_3\rangle @\text{U}(2)$ | 43 | $ f_{3x}\rangle @\text{U}(2)$ | 44 | $ f_{3y}\rangle @\text{U}(2)$ |
| 45 | $ f_{az}\rangle @\text{U}(2)$ | | | | | | | | |

Table 4: Atomic basis (orbital part only)

| orbital | definition |
|------------------|--|
| $ p_x\rangle$ | x |
| $ p_y\rangle$ | y |
| $ p_z\rangle$ | z |
| $ d_v\rangle$ | $\frac{\sqrt{3}(x^2 - y^2)}{2}$ |
| $ d_{xy}\rangle$ | $\sqrt{3}xy$ |
| $ d_{xz}\rangle$ | $\sqrt{3}xz$ |
| $ d_{yz}\rangle$ | $\sqrt{3}yz$ |
| $ d_u\rangle$ | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| $ f_2\rangle$ | $\frac{\sqrt{10}x(x^2 - 3y^2)}{4}$ |
| $ f_1\rangle$ | $\frac{\sqrt{10}y(3x^2 - y^2)}{4}$ |
| $ f_{bz}\rangle$ | $\frac{\sqrt{15}z(x^2 - y^2)}{2}$ |

continued ...

Table 4

| orbital | definition |
|------------------|--------------------------------------|
| $ f_3\rangle$ | $\sqrt{15}xyz$ |
| $ f_{3x}\rangle$ | $\frac{\sqrt{6}x(-x^2-y^2+4z^2)}{4}$ |
| $ f_{3y}\rangle$ | $\frac{\sqrt{6}y(-x^2-y^2+4z^2)}{4}$ |
| $ f_{az}\rangle$ | $\frac{z(-3x^2-3y^2+2z^2)}{2}$ |

SAMB: 380 (all 380)

• Pt1 : 'Pt1' site-cluster

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

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

* wyckoff: **2a**

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

$$\boxed{\text{z2}} \quad \mathbb{Q}_2^{(c)}(A_{1g}) = \mathbb{Q}_2^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

• **Pt2** : 'Pt2' site-cluster

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

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

* wyckoff: **2c**

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

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

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

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

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

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

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

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

$$\begin{aligned}
\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}
\end{aligned}$$

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

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

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

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

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

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

• **Si1** : 'Si1' site-cluster

* 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 : 'Si2' site-cluster

* 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** : 'U' site-cluster

* bra: $\langle f_2|, \langle f_1|, \langle f_{bz}|, \langle f_3|, \langle f_{3x}|, \langle f_{3y}|, \langle f_{az}|$

* ket: $|f_2\rangle, |f_1\rangle, |f_{bz}\rangle, |f_3\rangle, |f_{3x}\rangle, |f_{3y}\rangle, |f_{az}\rangle$

* wyckoff: 2c

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned}
\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}
\end{aligned}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

* wyckoff: **8a@8i**

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned}
\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}
\end{aligned}$$

$$\begin{aligned}
\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} \\
\text{z162} \quad \mathbb{Q}_2^{(c)}(B_{1g}, b) &= \mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_3^{(b)}(B_{2u}) \\
\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} \\
\text{z164} \quad \mathbb{Q}_2^{(c)}(B_{1g}, d) &= -\mathbb{Q}_3^{(a)}(A_{2u})\mathbb{Q}_3^{(b)}(B_{2u}) \\
\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} \\
\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{G}_{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} \\
\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} \\
\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} \\
\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} \\
\text{z170} \quad \mathbb{Q}_3^{(c)}(B_{1u}, b) &= \mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g}) \\
\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} \\
\text{z172} \quad \mathbb{Q}_3^{(c)}(B_{1u}, d) &= \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{1g}) \\
\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} \\
\text{z174} \quad \mathbb{G}_2^{(c)}(B_{1u}, a) &= \mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g}) \\
\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}
\end{aligned}$$

$$\begin{aligned}
\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} \\
\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} \\
\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} \\
\text{z179} \quad \mathbb{Q}_2^{(c)}(B_{2g}, d) &= \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_3^{(b)}(B_{2u}) \\
\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} \\
\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} \\
\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} \\
\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} \\
\text{z184} \quad \mathbb{Q}_3^{(c)}(B_{2u}, b) &= \mathbb{Q}_3^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g}) \\
\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} \\
\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} \\
\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} \\
\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} \\
\text{z189} \quad \mathbb{G}_2^{(c)}(B_{2u}, c) &= \mathbb{G}_2^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})
\end{aligned}$$

$$\begin{aligned}
\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}_{1,1}^{(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}
\end{aligned}$$

$$\begin{aligned}
\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}
\end{aligned}$$

$$\begin{aligned}
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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}
\end{aligned}$$

$$\begin{aligned}
\text{z362} \quad \mathbb{Q}_{3,2}^{(c)}(Eu, 1b) &= \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(Eu, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z363} \quad \mathbb{Q}_{3,1}^{(c)}(Eu, 1c) &= \frac{33\sqrt{1834}\mathbb{Q}_{3,1}^{(a)}(Eu, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{3668} + \frac{17\sqrt{27510}\mathbb{Q}_{3,1}^{(a)}(Eu, 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} \\
\text{z364} \quad \mathbb{Q}_{3,2}^{(c)}(Eu, 1c) &= -\frac{33\sqrt{1834}\mathbb{Q}_{3,2}^{(a)}(Eu, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{3668} - \frac{17\sqrt{27510}\mathbb{Q}_{3,2}^{(a)}(Eu, 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} \\
\text{z365} \quad \mathbb{Q}_{3,1}^{(c)}(Eu, 1d) &= -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(Eu)\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} \\
\text{z366} \quad \mathbb{Q}_{3,2}^{(c)}(Eu, 1d) &= \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(Eu)\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} \\
\text{z367} \quad \mathbb{Q}_{3,1}^{(c)}(Eu, 2a) &= \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(Eu, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z368} \quad \mathbb{Q}_{3,2}^{(c)}(Eu, 2a) &= \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(Eu, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z369} \quad \mathbb{Q}_{3,1}^{(c)}(Eu, 2b) &= \frac{25\sqrt{655}\mathbb{Q}_{3,1}^{(a)}(Eu, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} - \frac{5\sqrt{393}\mathbb{Q}_{3,1}^{(a)}(Eu, 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} \\
\text{z370} \quad \mathbb{Q}_{3,2}^{(c)}(Eu, 2b) &= -\frac{25\sqrt{655}\mathbb{Q}_{3,2}^{(a)}(Eu, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} + \frac{5\sqrt{393}\mathbb{Q}_{3,2}^{(a)}(Eu, 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} \\
\text{z371} \quad \mathbb{Q}_{3,1}^{(c)}(Eu, 2c) &= \frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(Eu)\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} \\
\text{z372} \quad \mathbb{Q}_{3,2}^{(c)}(Eu, 2c) &= -\frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(Eu)\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} \\
\text{z373} \quad \mathbb{Q}_{5,1}^{(c)}(Eu, 1) &= \frac{5\mathbb{Q}_{3,1}^{(a)}(Eu, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{16} - \frac{\sqrt{15}\mathbb{Q}_{3,1}^{(a)}(Eu, 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} \\
\text{z374} \quad \mathbb{Q}_{5,2}^{(c)}(Eu, 1) &= -\frac{5\mathbb{Q}_{3,2}^{(a)}(Eu, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{16} + \frac{\sqrt{15}\mathbb{Q}_{3,2}^{(a)}(Eu, 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} \\
\text{z375} \quad \mathbb{Q}_{5,1}^{(c)}(Eu, 2) &= -\frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(Eu, 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}
\end{aligned}$$

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

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

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

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

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

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

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

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

* wyckoff: **8a08i**

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

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

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

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

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

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

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

$$\begin{aligned}
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\text{z43} \quad \mathbb{G}_2^{(c)}(A_{1u}, c) &= \mathbb{G}_2^{(a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g}) \\
\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} \\
\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} \\
\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} \\
\text{z64} \quad \mathbb{Q}_4^{(c)}(A_{2g}, b) &= \mathbb{Q}_3^{(a)}(B_{1u})\mathbb{Q}_3^{(b)}(B_{2u}) \\
\text{z65} \quad \mathbb{Q}_4^{(c)}(A_{2g}, c) &= -\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_3^{(b)}(B_{2u}) \\
\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} \\
\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} \\
\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}
\end{aligned}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned}
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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}
\end{aligned}$$

$$\begin{aligned}
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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} \\
\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}
\end{aligned}$$

$$\begin{aligned}
\text{z324} \quad \mathbb{Q}_{1,2}^{(c)}(Eu, b) &= -\frac{\mathbb{Q}_{1,2}^{(a)}(Eu)\mathbb{Q}_2^{(b)}(B_{1g})}{2} + \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} \\
\text{z325} \quad \mathbb{Q}_{1,1}^{(c)}(Eu, c) &= \frac{3\sqrt{14}\mathbb{Q}_{3,1}^{(a)}(Eu, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{28} - \frac{\sqrt{210}\mathbb{Q}_{3,1}^{(a)}(Eu, 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} \\
\text{z326} \quad \mathbb{Q}_{1,2}^{(c)}(Eu, c) &= -\frac{3\sqrt{14}\mathbb{Q}_{3,2}^{(a)}(Eu, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{28} + \frac{\sqrt{210}\mathbb{Q}_{3,2}^{(a)}(Eu, 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} \\
\text{z327} \quad \mathbb{Q}_{1,1}^{(c)}(Eu, d) &= \frac{\sqrt{3}\mathbb{G}_{2,1}^{(a)}(Eu)\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} \\
\text{z328} \quad \mathbb{Q}_{1,2}^{(c)}(Eu, d) &= -\frac{\sqrt{3}\mathbb{G}_{2,2}^{(a)}(Eu)\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} \\
\text{z329} \quad \mathbb{Q}_{3,1}^{(c)}(Eu, 1a) &= \frac{\mathbb{Q}_{1,1}^{(a)}(Eu)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\text{z330} \quad \mathbb{Q}_{3,2}^{(c)}(Eu, 1a) &= -\frac{\mathbb{Q}_{1,2}^{(a)}(Eu)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{Q}_1^{(a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} \\
\text{z331} \quad \mathbb{Q}_{3,1}^{(c)}(Eu, 1b) &= \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(Eu, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z332} \quad \mathbb{Q}_{3,2}^{(c)}(Eu, 1b) &= \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(Eu, 1)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z333} \quad \mathbb{Q}_{3,1}^{(c)}(Eu, 1c) &= \frac{33\sqrt{1834}\mathbb{Q}_{3,1}^{(a)}(Eu, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{3668} + \frac{17\sqrt{27510}\mathbb{Q}_{3,1}^{(a)}(Eu, 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} \\
\text{z334} \quad \mathbb{Q}_{3,2}^{(c)}(Eu, 1c) &= -\frac{33\sqrt{1834}\mathbb{Q}_{3,2}^{(a)}(Eu, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{3668} - \frac{17\sqrt{27510}\mathbb{Q}_{3,2}^{(a)}(Eu, 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} \\
\text{z335} \quad \mathbb{Q}_{3,1}^{(c)}(Eu, 1d) &= -\frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(Eu)\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} \\
\text{z336} \quad \mathbb{Q}_{3,2}^{(c)}(Eu, 1d) &= \frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(Eu)\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} \\
\text{z337} \quad \mathbb{Q}_{3,1}^{(c)}(Eu, 2a) &= \frac{\sqrt{2}\mathbb{Q}_{3,1}^{(a)}(Eu, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2}
\end{aligned}$$

$$\begin{aligned}
\text{z338} \quad \mathbb{Q}_{3,2}^{(c)}(Eu, 2a) &= \frac{\sqrt{2}\mathbb{Q}_{3,2}^{(a)}(Eu, 2)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z339} \quad \mathbb{Q}_{3,1}^{(c)}(Eu, 2b) &= \frac{25\sqrt{655}\mathbb{Q}_{3,1}^{(a)}(Eu, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} - \frac{5\sqrt{393}\mathbb{Q}_{3,1}^{(a)}(Eu, 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} \\
\text{z340} \quad \mathbb{Q}_{3,2}^{(c)}(Eu, 2b) &= -\frac{25\sqrt{655}\mathbb{Q}_{3,2}^{(a)}(Eu, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{2096} + \frac{5\sqrt{393}\mathbb{Q}_{3,2}^{(a)}(Eu, 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} \\
\text{z341} \quad \mathbb{Q}_{3,1}^{(c)}(Eu, 2c) &= \frac{\sqrt{15}\mathbb{G}_{2,1}^{(a)}(Eu)\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} \\
\text{z342} \quad \mathbb{Q}_{3,2}^{(c)}(Eu, 2c) &= -\frac{\sqrt{15}\mathbb{G}_{2,2}^{(a)}(Eu)\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} \\
\text{z343} \quad \mathbb{Q}_{5,1}^{(c)}(Eu, 1) &= \frac{5\mathbb{Q}_{3,1}^{(a)}(Eu, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{16} - \frac{\sqrt{15}\mathbb{Q}_{3,1}^{(a)}(Eu, 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} \\
\text{z344} \quad \mathbb{Q}_{5,2}^{(c)}(Eu, 1) &= -\frac{5\mathbb{Q}_{3,2}^{(a)}(Eu, 1)\mathbb{Q}_2^{(b)}(B_{1g})}{16} + \frac{\sqrt{15}\mathbb{Q}_{3,2}^{(a)}(Eu, 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} \\
\text{z345} \quad \mathbb{Q}_{5,1}^{(c)}(Eu, 2) &= -\frac{\sqrt{10}\mathbb{Q}_{3,1}^{(a)}(Eu, 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} \\
\text{z346} \quad \mathbb{Q}_{5,2}^{(c)}(Eu, 2) &= \frac{\sqrt{10}\mathbb{Q}_{3,2}^{(a)}(Eu, 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} \\
\text{z347} \quad \mathbb{G}_{2,1}^{(c)}(Eu, a) &= \frac{\sqrt{2}\mathbb{G}_{2,1}^{(a)}(Eu)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z348} \quad \mathbb{G}_{2,2}^{(c)}(Eu, a) &= \frac{\sqrt{2}\mathbb{G}_{2,2}^{(a)}(Eu)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\text{z349} \quad \mathbb{G}_{2,1}^{(c)}(Eu, b) &= -\frac{\mathbb{G}_{2,1}^{(a)}(Eu)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} \\
\text{z350} \quad \mathbb{G}_{2,2}^{(c)}(Eu, b) &= \frac{\mathbb{G}_{2,2}^{(a)}(Eu)\mathbb{Q}_2^{(b)}(B_{1g})}{2} - \frac{\mathbb{G}_2^{(a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}
\end{aligned}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- bra: $\langle f_2|, \langle f_1|, \langle f_{bz}|, \langle f_3|, \langle f_{3x}|, \langle f_{3y}|, \langle f_{az}|$
- ket: $|f_2\rangle, |f_1\rangle, |f_{bz}\rangle, |f_3\rangle, |f_{3x}\rangle, |f_{3y}\rangle, |f_{az}\rangle$

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

$$\boxed{\text{x36}} \quad \mathbb{Q}_2^{(a)}(A_{1g}) = \begin{bmatrix} -\frac{5\sqrt{21}}{42} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{5\sqrt{21}}{42} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{21}}{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{21}}{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{21}}{21} \end{bmatrix}$$

$$\boxed{\text{x37}} \quad \mathbb{Q}_4^{(a)}(A_{1g}, 1) = \begin{bmatrix} \frac{\sqrt{66}}{44} & 0 & 0 & 0 & -\frac{\sqrt{110}}{44} & 0 & 0 \\ 0 & \frac{\sqrt{66}}{44} & 0 & 0 & 0 & \frac{\sqrt{110}}{44} & 0 \\ 0 & 0 & -\frac{\sqrt{66}}{66} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{66}}{11} & 0 & 0 & 0 \\ -\frac{\sqrt{110}}{44} & 0 & 0 & 0 & \frac{\sqrt{66}}{132} & 0 & 0 \\ 0 & \frac{\sqrt{110}}{44} & 0 & 0 & 0 & \frac{\sqrt{66}}{132} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{66}}{22} \end{bmatrix}$$

$$\boxed{\text{x38}} \quad \mathbb{Q}_4^{(a)}(A_{1g}, 2) = \begin{bmatrix} \frac{\sqrt{2310}}{308} & 0 & 0 & 0 & \frac{\sqrt{154}}{44} & 0 & 0 \\ 0 & \frac{\sqrt{2310}}{308} & 0 & 0 & 0 & -\frac{\sqrt{154}}{44} & 0 \\ 0 & 0 & -\frac{\sqrt{2310}}{66} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{154}}{44} & 0 & 0 & 0 & \frac{\sqrt{2310}}{924} & 0 & 0 \\ 0 & -\frac{\sqrt{154}}{44} & 0 & 0 & 0 & \frac{\sqrt{2310}}{924} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2310}}{154} \end{bmatrix}$$

$$\boxed{\text{x39}} \quad \mathbb{Q}_6^{(a)}(A_{1g}, 1) = \begin{bmatrix} -\frac{\sqrt{462}}{1848} & 0 & 0 & 0 & -\frac{\sqrt{770}}{88} & 0 & 0 \\ 0 & -\frac{\sqrt{462}}{1848} & 0 & 0 & 0 & \frac{\sqrt{770}}{88} & 0 \\ 0 & 0 & -\frac{3\sqrt{462}}{154} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{462}}{77} & 0 & 0 & 0 \\ -\frac{\sqrt{770}}{88} & 0 & 0 & 0 & -\frac{5\sqrt{462}}{616} & 0 & 0 \\ 0 & \frac{\sqrt{770}}{88} & 0 & 0 & 0 & -\frac{5\sqrt{462}}{616} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{5\sqrt{462}}{462} \end{bmatrix}$$

$$\boxed{\text{x40}} \quad \mathbb{Q}_6^{(a)}(A_{1g}, 2) = \begin{bmatrix} -\frac{\sqrt{66}}{264} & 0 & 0 & 0 & \frac{\sqrt{110}}{88} & 0 & 0 \\ 0 & -\frac{\sqrt{66}}{264} & 0 & 0 & 0 & -\frac{\sqrt{110}}{88} & 0 \\ 0 & 0 & \frac{\sqrt{66}}{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{110}}{88} & 0 & 0 & 0 & -\frac{5\sqrt{66}}{88} & 0 & 0 \\ 0 & -\frac{\sqrt{110}}{88} & 0 & 0 & 0 & -\frac{5\sqrt{66}}{88} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{5\sqrt{66}}{66} \end{bmatrix}$$

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

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

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

$$\boxed{\text{x44}} \quad \mathbb{Q}_4^{(a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & -\frac{3\sqrt{462}}{154} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{3\sqrt{462}}{154} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{462}}{154} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{3\sqrt{462}}{154} & 0 & 0 & 0 & -\frac{\sqrt{770}}{77} & 0 & 0 \\ 0 & -\frac{3\sqrt{462}}{154} & 0 & 0 & 0 & \frac{\sqrt{770}}{77} & 0 \\ 0 & 0 & \frac{\sqrt{462}}{154} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x45}} \quad \mathbb{Q}_6^{(a)}(B_{1g}, 1) = \begin{bmatrix} \frac{\sqrt{10}}{8} & 0 & 0 & 0 & \frac{\sqrt{6}}{24} & 0 & 0 \\ 0 & -\frac{\sqrt{10}}{8} & 0 & 0 & 0 & \frac{\sqrt{6}}{24} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}}{24} & 0 & 0 & 0 & -\frac{\sqrt{10}}{8} & 0 & 0 \\ 0 & \frac{\sqrt{6}}{24} & 0 & 0 & 0 & \frac{\sqrt{10}}{8} & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x46}} \quad \mathbb{Q}_6^{(a)}(B_{1g}, 2) = \begin{bmatrix} \frac{\sqrt{22}}{8} & 0 & 0 & 0 & -\frac{\sqrt{330}}{264} & 0 & 0 \\ 0 & -\frac{\sqrt{22}}{8} & 0 & 0 & 0 & -\frac{\sqrt{330}}{264} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{330}}{66} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{330}}{264} & 0 & 0 & 0 & \frac{5\sqrt{22}}{88} & 0 & 0 \\ 0 & -\frac{\sqrt{330}}{264} & 0 & 0 & 0 & -\frac{5\sqrt{22}}{88} & 0 \\ 0 & 0 & \frac{\sqrt{330}}{66} & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x47}} \quad \mathbb{Q}_2^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{105}}{42} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{105}}{42} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{105}}{21} \\ 0 & -\frac{\sqrt{105}}{42} & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 \\ \frac{\sqrt{105}}{42} & 0 & 0 & 0 & \frac{\sqrt{7}}{7} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{105}}{21} & 0 & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{\text{x50}} \quad \mathbb{Q}_6^{(a)}(B_{2g}, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{66}}{66} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{66}}{66} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{2\sqrt{66}}{33} \\ 0 & -\frac{\sqrt{66}}{66} & 0 & 0 & 0 & \frac{\sqrt{110}}{22} & 0 \\ \frac{\sqrt{66}}{66} & 0 & 0 & 0 & \frac{\sqrt{110}}{22} & 0 & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{66}}{33} & 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x51}} \quad \mathbb{Q}_{2,1}^{(a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & -\frac{5\sqrt{42}}{84} & 0 & 0 & 0 \\ 0 & 0 & \frac{5\sqrt{42}}{84} & 0 & 0 & 0 & 0 \\ 0 & \frac{5\sqrt{42}}{84} & 0 & 0 & 0 & -\frac{\sqrt{70}}{28} & 0 \\ -\frac{5\sqrt{42}}{84} & 0 & 0 & 0 & \frac{\sqrt{70}}{28} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{70}}{28} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{70}}{28} & 0 & 0 & 0 & \frac{\sqrt{42}}{42} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{42} & 0 \end{bmatrix}$$

$$\boxed{\text{x52}} \quad \mathbb{Q}_{2,2}^{(a)}(E_g) = \begin{bmatrix} 0 & 0 & \frac{5\sqrt{42}}{84} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{5\sqrt{42}}{84} & 0 & 0 & 0 \\ \frac{5\sqrt{42}}{84} & 0 & 0 & 0 & \frac{\sqrt{70}}{28} & 0 & 0 \\ 0 & \frac{5\sqrt{42}}{84} & 0 & 0 & 0 & \frac{\sqrt{70}}{28} & 0 \\ 0 & 0 & \frac{\sqrt{70}}{28} & 0 & 0 & 0 & \frac{\sqrt{42}}{42} \\ 0 & 0 & 0 & \frac{\sqrt{70}}{28} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{42}}{42} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x53}} \quad \mathbb{Q}_{4,1}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{165}}{44} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{165}}{44} & 0 & 0 & 0 & \frac{3\sqrt{11}}{44} \\ 0 & \frac{\sqrt{165}}{44} & 0 & 0 & 0 & \frac{3\sqrt{11}}{44} & 0 \\ -\frac{\sqrt{165}}{44} & 0 & 0 & 0 & -\frac{5\sqrt{11}}{44} & 0 & 0 \\ 0 & 0 & 0 & -\frac{5\sqrt{11}}{44} & 0 & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{11}}{44} & 0 & 0 & 0 & -\frac{\sqrt{165}}{44} \\ 0 & \frac{3\sqrt{11}}{44} & 0 & 0 & 0 & -\frac{\sqrt{165}}{44} & 0 \end{bmatrix}$$

$$\boxed{\text{x54}} \quad \mathbb{Q}_{4,2}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{165}}{44} & 0 & 0 & 0 & -\frac{3\sqrt{11}}{44} \\ 0 & 0 & 0 & \frac{\sqrt{165}}{44} & 0 & 0 & 0 \\ \frac{\sqrt{165}}{44} & 0 & 0 & 0 & -\frac{3\sqrt{11}}{44} & 0 & 0 \\ 0 & \frac{\sqrt{165}}{44} & 0 & 0 & 0 & -\frac{5\sqrt{11}}{44} & 0 \\ 0 & 0 & -\frac{3\sqrt{11}}{44} & 0 & 0 & 0 & -\frac{\sqrt{165}}{44} \\ 0 & 0 & 0 & -\frac{5\sqrt{11}}{44} & 0 & 0 & 0 \\ -\frac{3\sqrt{11}}{44} & 0 & 0 & 0 & -\frac{\sqrt{165}}{44} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x55}} \quad \mathbb{Q}_{4,1}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{1155}}{308} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{1155}}{308} & 0 & 0 & 0 & -\frac{3\sqrt{77}}{44} \\ 0 & \frac{\sqrt{1155}}{308} & 0 & 0 & 0 & \frac{\sqrt{77}}{28} & 0 \\ -\frac{\sqrt{1155}}{308} & 0 & 0 & 0 & \frac{3\sqrt{77}}{308} & 0 & 0 \\ 0 & 0 & 0 & \frac{3\sqrt{77}}{308} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{77}}{28} & 0 & 0 & 0 & -\frac{\sqrt{1155}}{308} \\ 0 & -\frac{3\sqrt{77}}{44} & 0 & 0 & 0 & -\frac{\sqrt{1155}}{308} & 0 \end{bmatrix}$$

$$\boxed{\text{x56}} \quad \mathbb{Q}_{4,2}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{1155}}{308} & 0 & 0 & 0 & \frac{3\sqrt{77}}{44} \\ 0 & 0 & 0 & \frac{\sqrt{1155}}{308} & 0 & 0 & 0 \\ \frac{\sqrt{1155}}{308} & 0 & 0 & 0 & -\frac{\sqrt{77}}{28} & 0 & 0 \\ 0 & \frac{\sqrt{1155}}{308} & 0 & 0 & 0 & \frac{3\sqrt{77}}{308} & 0 \\ 0 & 0 & -\frac{\sqrt{77}}{28} & 0 & 0 & 0 & -\frac{\sqrt{1155}}{308} \\ 0 & 0 & 0 & \frac{3\sqrt{77}}{308} & 0 & 0 & 0 \\ \frac{3\sqrt{77}}{44} & 0 & 0 & 0 & -\frac{\sqrt{1155}}{308} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x57}} \quad \mathbb{Q}_{6,1}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & -\frac{3\sqrt{22}}{44} & 0 & 0 & 0 \\ 0 & 0 & -\frac{5\sqrt{22}}{88} & 0 & 0 & 0 & -\frac{\sqrt{330}}{88} \\ 0 & -\frac{5\sqrt{22}}{88} & 0 & 0 & 0 & -\frac{\sqrt{330}}{88} & 0 \\ -\frac{3\sqrt{22}}{44} & 0 & 0 & 0 & -\frac{\sqrt{330}}{44} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{330}}{44} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{330}}{88} & 0 & 0 & 0 & \frac{5\sqrt{22}}{88} \\ 0 & -\frac{\sqrt{330}}{88} & 0 & 0 & 0 & \frac{5\sqrt{22}}{88} & 0 \end{bmatrix}$$

$$\boxed{\text{x58}} \quad \mathbb{Q}_{6,2}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & -\frac{5\sqrt{22}}{88} & 0 & 0 & 0 & \frac{\sqrt{330}}{88} \\ 0 & 0 & 0 & \frac{3\sqrt{22}}{44} & 0 & 0 & 0 \\ -\frac{5\sqrt{22}}{88} & 0 & 0 & 0 & \frac{\sqrt{330}}{88} & 0 & 0 \\ 0 & \frac{3\sqrt{22}}{44} & 0 & 0 & 0 & -\frac{\sqrt{330}}{44} & 0 \\ 0 & 0 & \frac{\sqrt{330}}{88} & 0 & 0 & 0 & \frac{5\sqrt{22}}{88} \\ 0 & 0 & 0 & -\frac{\sqrt{330}}{44} & 0 & 0 & 0 \\ \frac{\sqrt{330}}{88} & 0 & 0 & 0 & \frac{5\sqrt{22}}{88} & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{\text{x61}} \quad \mathbb{Q}_{6,1}^{(a)}(E_g, 3) = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{165}}{33} & 0 & 0 & 0 \\ 0 & 0 & \frac{17\sqrt{165}}{528} & 0 & 0 & 0 & -\frac{9\sqrt{11}}{176} \\ 0 & \frac{17\sqrt{165}}{528} & 0 & 0 & 0 & -\frac{\sqrt{11}}{16} & 0 \\ \frac{\sqrt{165}}{33} & 0 & 0 & 0 & -\frac{\sqrt{11}}{11} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{11}}{11} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{11}}{16} & 0 & 0 & 0 & \frac{5\sqrt{165}}{528} \\ 0 & -\frac{9\sqrt{11}}{176} & 0 & 0 & 0 & \frac{5\sqrt{165}}{528} & 0 \end{bmatrix}$$

$$\boxed{\text{x62}} \quad \mathbb{Q}_{6,2}^{(a)}(E_g, 3) = \begin{bmatrix} 0 & 0 & \frac{17\sqrt{165}}{528} & 0 & 0 & 0 & \frac{9\sqrt{11}}{176} \\ 0 & 0 & 0 & -\frac{\sqrt{165}}{33} & 0 & 0 & 0 \\ \frac{17\sqrt{165}}{528} & 0 & 0 & 0 & \frac{\sqrt{11}}{16} & 0 & 0 \\ 0 & -\frac{\sqrt{165}}{33} & 0 & 0 & 0 & -\frac{\sqrt{11}}{11} & 0 \\ 0 & 0 & \frac{\sqrt{11}}{16} & 0 & 0 & 0 & \frac{5\sqrt{165}}{528} \\ 0 & 0 & 0 & -\frac{\sqrt{11}}{11} & 0 & 0 & 0 \\ \frac{9\sqrt{11}}{176} & 0 & 0 & 0 & \frac{5\sqrt{165}}{528} & 0 & 0 \end{bmatrix}$$

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

$$\boxed{\text{x64}} \quad \mathbb{M}_1^{(a)}(A_{2g}) = \begin{bmatrix} 0 & -\frac{3\sqrt{7}i}{14} & 0 & 0 & 0 & 0 & 0 \\ \frac{3\sqrt{7}i}{14} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{7}i}{7} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{7}i}{7} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{7}i}{14} & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{7}i}{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

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

$$\boxed{\text{x66}} \quad \mathbb{M}_5^{(a)}(A_{2g}, 1) = \begin{bmatrix} 0 & -\frac{\sqrt{21}i}{42} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{21}i}{42} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{2\sqrt{21}i}{21} & 0 & 0 & 0 \\ 0 & 0 & -\frac{2\sqrt{21}i}{21} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{5\sqrt{21}i}{42} & 0 \\ 0 & 0 & 0 & 0 & \frac{5\sqrt{21}i}{42} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

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

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

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

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

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

$$\boxed{\text{x72}} \quad \mathbb{M}_{1,1}^{(a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{42}i}{28} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{42}i}{28} & 0 & 0 & 0 & \frac{\sqrt{70}i}{28} & 0 \\ -\frac{\sqrt{42}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{70}i}{28} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{70}i}{28} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{70}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}i}{14} \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{42}i}{14} & 0 \end{bmatrix}$$

$$\boxed{\text{x73}} \quad \mathbb{M}_{1,2}^{(a)}(E_g) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{42}i}{28} & 0 & 0 & 0 \\ \frac{\sqrt{42}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{70}i}{28} & 0 & 0 \\ 0 & \frac{\sqrt{42}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{70}i}{28} & 0 \\ 0 & 0 & \frac{\sqrt{70}i}{28} & 0 & 0 & 0 & -\frac{\sqrt{42}i}{14} \\ 0 & 0 & 0 & \frac{\sqrt{70}i}{28} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{42}i}{14} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x74}} \quad \mathbb{M}_{3,1}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & \frac{i}{4} & 0 & 0 & 0 \\ 0 & 0 & -\frac{i}{4} & 0 & 0 & 0 & \frac{\sqrt{15}i}{12} \\ 0 & \frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 \\ -\frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{4} \\ 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 & -\frac{i}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x75}} \quad \mathbb{M}_{3,2}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & -\frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} \\ 0 & 0 & 0 & -\frac{i}{4} & 0 & 0 & 0 \\ \frac{i}{4} & 0 & 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 \\ 0 & \frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{4} \\ 0 & 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 \\ \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & -\frac{i}{4} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x76}} \quad \mathbb{M}_{3,1}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 & -\frac{i}{4} \\ 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{4} & 0 \\ -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{4} & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{4} & 0 & 0 & 0 \\ 0 & 0 & -\frac{i}{4} & 0 & 0 & 0 & \frac{\sqrt{15}i}{12} \\ 0 & \frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 \end{bmatrix}$$

$$\boxed{\text{x77}} \quad \mathbb{M}_{3,2}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 & 0 \\ \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & -\frac{i}{4} & 0 & 0 \\ 0 & \frac{\sqrt{15}i}{12} & 0 & 0 & 0 & \frac{i}{4} & 0 \\ 0 & 0 & \frac{i}{4} & 0 & 0 & 0 & \frac{\sqrt{15}i}{12} \\ 0 & 0 & 0 & -\frac{i}{4} & 0 & 0 & 0 \\ -\frac{i}{4} & 0 & 0 & 0 & -\frac{\sqrt{15}i}{12} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x78}} \quad \mathbb{M}_{5,1}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{14}i}{14} & 0 & 0 & 0 \\ 0 & 0 & -\frac{13\sqrt{14}i}{112} & 0 & 0 & 0 & \frac{\sqrt{210}i}{48} \\ 0 & \frac{13\sqrt{14}i}{112} & 0 & 0 & 0 & -\frac{\sqrt{210}i}{336} & 0 \\ \frac{\sqrt{14}i}{14} & 0 & 0 & 0 & \frac{\sqrt{210}i}{42} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{210}i}{42} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{210}i}{336} & 0 & 0 & 0 & -\frac{5\sqrt{14}i}{112} \\ 0 & -\frac{\sqrt{210}i}{48} & 0 & 0 & 0 & \frac{5\sqrt{14}i}{112} & 0 \end{bmatrix}$$

$$\boxed{\text{x79}} \quad \mathbb{M}_{5,2}^{(a)}(E_g, 1) = \begin{bmatrix} 0 & 0 & -\frac{13\sqrt{14}i}{112} & 0 & 0 & 0 & -\frac{\sqrt{210}i}{48} \\ 0 & 0 & 0 & \frac{\sqrt{14}i}{14} & 0 & 0 & 0 \\ \frac{13\sqrt{14}i}{112} & 0 & 0 & 0 & \frac{\sqrt{210}i}{336} & 0 & 0 \\ 0 & -\frac{\sqrt{14}i}{14} & 0 & 0 & 0 & \frac{\sqrt{210}i}{42} & 0 \\ 0 & 0 & -\frac{\sqrt{210}i}{336} & 0 & 0 & 0 & -\frac{5\sqrt{14}i}{112} \\ 0 & 0 & 0 & -\frac{\sqrt{210}i}{42} & 0 & 0 & 0 \\ \frac{\sqrt{210}i}{48} & 0 & 0 & 0 & \frac{5\sqrt{14}i}{112} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x80}} \quad \mathbb{M}_{5,1}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{10}i}{16} & 0 & 0 & 0 & -\frac{3\sqrt{6}i}{16} \\ 0 & \frac{\sqrt{10}i}{16} & 0 & 0 & 0 & -\frac{3\sqrt{6}i}{16} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{3\sqrt{6}i}{16} & 0 & 0 & 0 & -\frac{\sqrt{10}i}{16} \\ 0 & \frac{3\sqrt{6}i}{16} & 0 & 0 & 0 & \frac{\sqrt{10}i}{16} & 0 \end{bmatrix}$$

$$\boxed{\text{x81}} \quad \mathbb{M}_{5,2}^{(a)}(E_g, 2) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{10}i}{16} & 0 & 0 & 0 & \frac{3\sqrt{6}i}{16} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{10}i}{16} & 0 & 0 & 0 & \frac{3\sqrt{6}i}{16} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{3\sqrt{6}i}{16} & 0 & 0 & 0 & -\frac{\sqrt{10}i}{16} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{3\sqrt{6}i}{16} & 0 & 0 & 0 & \frac{\sqrt{10}i}{16} & 0 & 0 \end{bmatrix}$$

$$\begin{aligned}
\boxed{\text{x82}} \quad \mathbb{M}_{5,1}^{(a)}(E_g, 3) &= \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{30}i}{12} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{30}i}{24} & 0 & 0 & 0 & \frac{\sqrt{2}i}{8} \\ 0 & -\frac{\sqrt{30}i}{24} & 0 & 0 & 0 & -\frac{\sqrt{2}i}{8} & 0 \\ -\frac{\sqrt{30}i}{12} & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}i}{8} & 0 & 0 & 0 & -\frac{\sqrt{30}i}{24} \\ 0 & -\frac{\sqrt{2}i}{8} & 0 & 0 & 0 & \frac{\sqrt{30}i}{24} & 0 \end{bmatrix} \\
\boxed{\text{x83}} \quad \mathbb{M}_{5,2}^{(a)}(E_g, 3) &= \begin{bmatrix} 0 & 0 & \frac{\sqrt{30}i}{24} & 0 & 0 & 0 & -\frac{\sqrt{2}i}{8} \\ 0 & 0 & 0 & -\frac{\sqrt{30}i}{12} & 0 & 0 & 0 \\ -\frac{\sqrt{30}i}{24} & 0 & 0 & 0 & \frac{\sqrt{2}i}{8} & 0 & 0 \\ 0 & \frac{\sqrt{30}i}{12} & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{8} & 0 & 0 & 0 & -\frac{\sqrt{30}i}{24} \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ \frac{\sqrt{2}i}{8} & 0 & 0 & 0 & \frac{\sqrt{30}i}{24} & 0 & 0 \end{bmatrix}
\end{aligned}$$

Cluster SAMB

- Site cluster

** Wyckoff: 2a

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

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

** Wyckoff: 2b

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

$$\boxed{\text{y4}} \quad \mathbb{Q}_3^{(s)}(B_{2u}) = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

** Wyckoff: 2c

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

$$\boxed{\text{y6}} \quad \mathbb{Q}_1^{(s)}(A_{2u}) = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

• Bond cluster

** Wyckoff: 8a@8i

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Site and Bond

Table 5: Orbital of each site

| # | site | orbital |
|---|------|---|
| 1 | Pt1 | $ d_v\rangle, d_{xy}\rangle, d_{xz}\rangle, d_{yz}\rangle, d_u\rangle$ |
| 2 | Pt2 | $ d_v\rangle, d_{xy}\rangle, d_{xz}\rangle, d_{yz}\rangle, d_u\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_2\rangle, f_1\rangle, f_{bz}\rangle, f_3\rangle, f_{3x}\rangle, f_{3y}\rangle, f_{az}\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] |
| 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] |

continued ...

Table 13

| SL | vector (\boldsymbol{v}) | center (\boldsymbol{c}) | mapping | head | tail | \boldsymbol{R} (primitive) |
|----|------------------------------|------------------------------|---------|-------|-------|------------------------------|
| 8 | [-0.50000, 0.00000, 0.12150] | [0.00000, 0.75000, 0.56075] | [8,12] | (2,1) | (2,1) | [1,0,0] |