

Model for “C3v1”

Generated on 2026-01-25 20:44:23 by MultiPie 2.0.4

General Condition

- Basis type: **lgs**
- SAMB selection:
 - Type: [Q, G]
 - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
 - Irrep.: [A_1 , A_2 , E]
 - 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_1 , A_2 , E]
 - Spin (s): [0, 1]
- Site-cluster selection:
 - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
 - Irrep.: [A_1 , A_2 , E]
- Bond-cluster selection:
 - Type: [Q, G, M, T]
 - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
 - Irrep.: [A_1 , A_2 , E]
- Max. neighbor: 10
- Search cell range: (-2, 3), (-2, 3), (-2, 3)
- Toroidal priority: **false**

Group and Unit Cell

- Group: SG No. 156 C_{3v}^1 $P3m1$ [trigonal]
- Associated point group: PG No. 156 C_{3v} $3m$ (3m1 setting) [trigonal]
- Unit cell:
 - $a = 1.00000$, $b = 1.00000$, $c = 1.00000$, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 120.0$
- Lattice vectors (conventional cell):
 - $\mathbf{a}_1 = [1.00000, 0.00000, 0.00000]$
 - $\mathbf{a}_2 = [-0.50000, 0.86603, 0.00000]$
 - $\mathbf{a}_3 = [0.00000, 0.00000, 1.00000]$

Symmetry Operation

Table 1: Symmetry operation

| # | SO | # | SO | # | SO | # | SO | # | SO |
|---|-----------------|---|-------------------|---|-------------------|---|-----------------|---|-----------------|
| 1 | $\{1 0\}$ | 2 | $\{3_{001}^+ 0\}$ | 3 | $\{3_{001}^- 0\}$ | 4 | $\{m_{110} 0\}$ | 5 | $\{m_{100} 0\}$ |
| 6 | $\{m_{010} 0\}$ | | | | | | | | |

Harmonics

Table 2: Harmonics

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|---|------------------------|--------|------|--------|--------------|-----------|----------------------------------------|
| 1 | $\mathbb{Q}_0(A_1)$ | A_1 | 0 | Q, T | - | - | 1 |
| 2 | $\mathbb{Q}_1(A_1)$ | A_1 | 1 | Q, T | - | - | z |
| 3 | $\mathbb{Q}_2(A_1)$ | A_1 | 2 | Q, T | - | - | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| 4 | $\mathbb{G}_3(A_1)$ | A_1 | 3 | G, M | - | - | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$ |
| 5 | $\mathbb{Q}_3(A_1, 1)$ | A_1 | 3 | Q, T | 1 | - | $-\frac{z(3x^2+3y^2-2z^2)}{2}$ |
| 6 | $\mathbb{Q}_3(A_1, 2)$ | A_1 | 3 | Q, T | 2 | - | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$ |
| 7 | $\mathbb{G}_0(A_2)$ | A_2 | 0 | G, M | - | - | 1 |
| 8 | $\mathbb{G}_1(A_2)$ | A_2 | 1 | G, M | - | - | z |

continued ...

Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|----|--------------------------|--------|------|--------|--------------|-----------|------------------------------------------|
| 9 | $\mathbb{G}_2(A_2)$ | A_2 | 2 | G, M | - | - | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| 10 | $\mathbb{G}_3(A_2, 2)$ | A_2 | 3 | G, M | 2 | - | $\frac{\sqrt{10}y(3x^2 - y^2)}{4}$ |
| 11 | $\mathbb{Q}_3(A_2)$ | A_2 | 3 | Q, T | - | - | $\frac{\sqrt{10}x(x^2 - 3y^2)}{4}$ |
| 12 | $\mathbb{G}_{1,1}(E)$ | E | 1 | G, M | - | 1 | $-y$ |
| 13 | $\mathbb{G}_{1,2}(E)$ | | | | | 2 | x |
| 14 | $\mathbb{Q}_{1,1}(E)$ | E | 1 | Q, T | - | 1 | x |
| 15 | $\mathbb{Q}_{1,2}(E)$ | | | | | 2 | y |
| 16 | $\mathbb{G}_{2,1}(E, 2)$ | E | 2 | G, M | 2 | 1 | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| 17 | $\mathbb{G}_{2,2}(E, 2)$ | | | | | 2 | $-\sqrt{3}xy$ |
| 18 | $\mathbb{Q}_{2,1}(E, 1)$ | E | 2 | Q, T | 1 | 1 | $\sqrt{3}xz$ |
| 19 | $\mathbb{Q}_{2,2}(E, 1)$ | | | | | 2 | $\sqrt{3}yz$ |
| 20 | $\mathbb{Q}_{2,1}(E, 2)$ | E | 2 | Q, T | 2 | 1 | $\sqrt{3}xy$ |
| 21 | $\mathbb{Q}_{2,2}(E, 2)$ | | | | | 2 | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| 22 | $\mathbb{G}_{3,1}(E, 1)$ | E | 3 | G, M | 1 | 1 | $\frac{\sqrt{6}y(x^2 + y^2 - 4z^2)}{4}$ |
| 23 | $\mathbb{G}_{3,2}(E, 1)$ | | | | | 2 | $-\frac{\sqrt{6}x(x^2 + y^2 - 4z^2)}{4}$ |
| 24 | $\mathbb{G}_{3,1}(E, 2)$ | E | 3 | G, M | 2 | 1 | $-\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |
| 25 | $\mathbb{G}_{3,2}(E, 2)$ | | | | | 2 | $\sqrt{15}xyz$ |
| 26 | $\mathbb{Q}_{3,1}(E, 1)$ | E | 3 | Q, T | 1 | 1 | $-\frac{\sqrt{6}x(x^2 + y^2 - 4z^2)}{4}$ |
| 27 | $\mathbb{Q}_{3,2}(E, 1)$ | | | | | 2 | $-\frac{\sqrt{6}y(x^2 + y^2 - 4z^2)}{4}$ |
| 28 | $\mathbb{Q}_{3,1}(E, 2)$ | E | 3 | Q, T | 2 | 1 | $\sqrt{15}xyz$ |
| 29 | $\mathbb{Q}_{3,2}(E, 2)$ | | | | | 2 | $\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |

continued ...

Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|----|--------------------------|--------|------|--------|--------------|-----------|-------------------------------------------------|
| 30 | $\mathbb{G}_{4,1}(E, 2)$ | E | 4 | G, M | 2 | 1 | $\frac{\sqrt{35}(x^2-2xy-y^2)(x^2+2xy-y^2)}{8}$ |
| 31 | $\mathbb{G}_{4,2}(E, 2)$ | | | | | 2 | $\frac{\sqrt{35}xy(x-y)(x+y)}{2}$ |

Basis in full matrix

Table 3: dimension = 8

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

Table 4: Atomic basis (orbital part only)

| orbital | definition |
|----------------------|------------|
| $ p_x\rangle$ | x |
| $ p_y\rangle$ | y |
| <i>continued ...</i> | |

Table 4

| orbital | definition |
|---------------|------------|
| $ p_z\rangle$ | z |

SAMB

60 (all 60) SAMBs

• 'A' site-cluster : **A**

* bra: $\langle p_x, \uparrow |, \langle p_x, \downarrow |, \langle p_y, \uparrow |, \langle p_y, \downarrow |$

* ket: $|p_x, \uparrow\rangle, |p_x, \downarrow\rangle, |p_y, \uparrow\rangle, |p_y, \downarrow\rangle$

* wyckoff: **1b**

$$\boxed{\text{z1}} \quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$$

$$\boxed{\text{z2}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_1) = \mathbb{Q}_2^{(1,-1;a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$$

$$\boxed{\text{z21}} \quad \mathbb{Q}_{2,1}^{(c)}(E, 2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{\text{z22}} \quad \mathbb{Q}_{2,2}^{(c)}(E, 2) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{\text{z23}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E, 1) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E, 1)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{\text{z24}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E, 1) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E, 1)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

• 'B' site-cluster : **B**

* bra: $\langle p_x, \uparrow |, \langle p_x, \downarrow |, \langle p_y, \uparrow |, \langle p_y, \downarrow |$

* ket: $|p_x, \uparrow\rangle, |p_x, \downarrow\rangle, |p_y, \uparrow\rangle, |p_y, \downarrow\rangle$

* wyckoff: 1c

$$\boxed{\text{z3}} \quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$$

$$\boxed{\text{z4}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_1) = \mathbb{Q}_2^{(1,-1;a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$$

$$\boxed{\text{z25}} \quad \mathbb{Q}_{2,1}^{(c)}(E, 2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{\text{z26}} \quad \mathbb{Q}_{2,2}^{(c)}(E, 2) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{\text{z27}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E, 1) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E, 1)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{\text{z28}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E, 1) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E, 1)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

• 'A'-'B' bond-cluster : B;A_001_1

* bra: $\langle p_x, \uparrow |, \langle p_x, \downarrow |, \langle p_y, \uparrow |, \langle p_y, \downarrow |$

* ket: $|p_x, \uparrow \rangle, |p_x, \downarrow \rangle, |p_y, \uparrow \rangle, |p_y, \downarrow \rangle$

* wyckoff: 3a03d

$$\boxed{\text{z5}} \quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(b)}(A_1)$$

$$\boxed{\text{z6}} \quad \mathbb{Q}_3^{(c)}(A_1, 2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z7}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_1, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E, 1)\mathbb{Q}_{1,1}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E, 1)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z8}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_1, b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z9}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_1) = \mathbb{Q}_2^{(1,-1;a)}(A_1)\mathbb{Q}_0^{(b)}(A_1)$$

$$\boxed{\text{z10}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_1, 1) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,1}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z11}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_1, 2) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 2)\mathbb{T}_{1,1}^{(b)}(E)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z12}} \quad \mathbb{G}_3^{(1,-1;c)}(A_1) = \mathbb{M}_3^{(1,-1;a)}(A_1)\mathbb{T}_0^{(b)}(A_1)$$

$$\boxed{\text{z13}} \quad \mathbb{Q}_3^{(c)}(A_2) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z14}} \quad \mathbb{Q}_3^{(1,-1;c)}(A_2) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 2)\mathbb{T}_{1,2}^{(b)}(E)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z15}} \quad \mathbb{G}_1^{(c)}(A_2) = \mathbb{M}_1^{(a)}(A_2)\mathbb{T}_0^{(b)}(A_1)$$

$$\boxed{\text{z16}} \quad \mathbb{G}_0^{(1,-1;c)}(A_2) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z17}} \quad \mathbb{G}_1^{(1,-1;c)}(A_2) = \mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_0^{(b)}(A_1)$$

$$\boxed{\text{z18}} \quad \mathbb{G}_2^{(1,-1;c)}(A_2, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E, 1)\mathbb{Q}_{1,2}^{(b)}(E)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E, 1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z19}} \quad \mathbb{G}_2^{(1,-1;c)}(A_2, b) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,2}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z20}} \quad \mathbb{G}_3^{(1,-1;c)}(A_2, 2) = \mathbb{M}_3^{(1,-1;a)}(A_2, 2)\mathbb{T}_0^{(b)}(A_1)$$

$$\boxed{\text{z29}} \quad \mathbb{Q}_{1,1}^{(c)}(E, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z30}} \quad \mathbb{Q}_{1,2}^{(c)}(E, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z31}} \quad \mathbb{Q}_{1,1}^{(c)}(E, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(b)}(E)}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z32}} \quad \mathbb{Q}_{1,2}^{(c)}(E, b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(b)}(E)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z33}} \quad \mathbb{Q}_{1,1}^{(c)}(E, c) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z34}} \quad \mathbb{Q}_{1,2}^{(c)}(E, c) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z35}} \quad \mathbb{Q}_{2,1}^{(c)}(E, 2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z36}} \quad \mathbb{Q}_{2,2}^{(c)}(E, 2) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z37}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E, a) = -\frac{\sqrt{2}\mathbb{Q}_2^{(1,-1;a)}(A_1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z38}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E, a) = -\frac{\sqrt{2}\mathbb{Q}_2^{(1,-1;a)}(A_1)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z39}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E, b) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z40}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E, b) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z41}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E, 1) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E, 1)\mathbb{Q}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z42}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E, 1) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E, 1)\mathbb{Q}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z43}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E, 1) = -\frac{\mathbb{M}_{3,1}^{(1,-1;a)}(E, 2)\mathbb{T}_{1,2}^{(b)}(E)}{2} - \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(E, 2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z44}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E, 1) = -\frac{\mathbb{M}_{3,1}^{(1,-1;a)}(E, 2)\mathbb{T}_{1,1}^{(b)}(E)}{2} + \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(E, 2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z45}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E, 2a) = \frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(E, 1)\mathbb{Q}_{1,2}^{(b)}(E)}{2} + \frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(E, 1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z46}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E, 2a) = \frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(E, 1)\mathbb{Q}_{1,1}^{(b)}(E)}{2} - \frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(E, 1)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z47}} \quad \mathbb{Q}_{3,1}^{(1,-1;c)}(E, 2b) = \frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,2}^{(b)}(E)}{8} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,1}^{(b)}(E)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(A_1)\mathbb{T}_{1,1}^{(b)}(E)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(A_2, 2)\mathbb{T}_{1,2}^{(b)}(E)}{8}$$

$$\boxed{\text{z48}} \quad \mathbb{Q}_{3,2}^{(1,-1;c)}(E, 2b) = \frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,1}^{(b)}(E)}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,2}^{(b)}(E)}{8} + \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(A_1)\mathbb{T}_{1,2}^{(b)}(E)}{8} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(A_2, 2)\mathbb{T}_{1,1}^{(b)}(E)}{8}$$

$$\boxed{\text{z49}} \quad \mathbb{G}_{1,1}^{(1,-1;c)}(E) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z50}} \quad \mathbb{G}_{1,2}^{(1,-1;c)}(E) = \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z51}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E, 2a) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,2}^{(b)}(E)}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,1}^{(b)}(E)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A_1)\mathbb{T}_{1,1}^{(b)}(E)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A_2, 2)\mathbb{T}_{1,2}^{(b)}(E)}{8}$$

$$\boxed{\text{z52}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E, 2a) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,1}^{(b)}(E)}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 1)\mathbb{T}_{1,2}^{(b)}(E)}{8} + \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A_1)\mathbb{T}_{1,2}^{(b)}(E)}{8} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(A_2, 2)\mathbb{T}_{1,1}^{(b)}(E)}{8}$$

$$\boxed{\text{z53}} \quad \mathbb{G}_{2,1}^{(1,-1;c)}(E, 2b) = \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2} + \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z54}} \quad \mathbb{G}_{2,2}^{(1,-1;c)}(E, 2b) = \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z55}} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(E, 1) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 1)\mathbb{T}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z56}} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(E, 1) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 1)\mathbb{T}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z57}} \quad \mathbb{G}_{3,1}^{(1,-1;c)}(E, 2) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E, 2)\mathbb{T}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z58}} \quad \mathbb{G}_{3,2}^{(1,-1;c)}(E, 2) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E, 2)\mathbb{T}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z59}} \quad \mathbb{G}_{4,1}^{(1,-1;c)}(E, 2) = \frac{\mathbb{M}_3^{(1,-1;a)}(A_1)\mathbb{T}_{1,1}^{(b)}(E)}{2} - \frac{\mathbb{M}_3^{(1,-1;a)}(A_2, 2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z60}} \quad \mathbb{G}_{4,2}^{(1,-1;c)}(E, 2) = \frac{\mathbb{M}_3^{(1,-1;a)}(A_1)\mathbb{T}_{1,2}^{(b)}(E)}{2} + \frac{\mathbb{M}_3^{(1,-1;a)}(A_2, 2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

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

$$\boxed{\text{x1}} \quad \mathbb{Q}_0^{(a)}(A_1) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

$$\boxed{\text{x2}} \quad \mathbb{Q}_{2,1}^{(a)}(E, 2) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x3}} \quad \mathbb{Q}_{2,2}^{(a)}(E, 2) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$$

$$\boxed{\text{x4}} \quad \mathbb{Q}_2^{(1,-1;a)}(A_1) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{\text{x7}} \quad \mathbb{M}_1^{(a)}(A_2) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x8}} \quad \mathbb{M}_3^{(1,-1;a)}(A_1) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x9}} \quad \mathbb{M}_1^{(1,-1;a)}(A_2) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$$

$$\boxed{\text{x10}} \quad \mathbb{M}_3^{(1,-1;a)}(A_2, 2) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x11}} \quad \mathbb{M}_{1,1}^{(1,-1;a)}(E) = \begin{bmatrix} 0 & \frac{i}{2} & 0 & 0 \\ -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ 0 & 0 & -\frac{i}{2} & 0 \end{bmatrix}$$

$$\boxed{\text{x12}} \quad \mathbb{M}_{1,2}^{(1,-1;a)}(E) = \begin{bmatrix} 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \end{bmatrix}$$

$$\boxed{\text{x13}} \quad \mathbb{M}_{3,1}^{(1,-1;a)}(E, 1) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x14}} \quad \mathbb{M}_{3,2}^{(1,-1;a)}(E, 1) = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} \\ -\frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$$\boxed{\text{x15}} \quad \mathbb{M}_{3,1}^{(1,-1;a)}(E, 2) = \begin{bmatrix} -\frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$$

$$\boxed{\text{x16}} \quad \mathbb{M}_{3,2}^{(1,-1;a)}(E,2) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \end{bmatrix}$$

Cluster SAMB

- Site cluster

** Wyckoff: 1c

$$\boxed{\text{y1}} \quad \mathbb{Q}_0^{(s)}(A_1) = [1]$$

** Wyckoff: 1b

$$\boxed{\text{y2}} \quad \mathbb{Q}_0^{(s)}(A_1) = [1]$$

- Bond cluster

** Wyckoff: 3a@3d

$$\boxed{\text{y3}} \quad \mathbb{Q}_0^{(s)}(A_1) = \left[\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3} \right]$$

$$\boxed{\text{y4}} \quad \mathbb{T}_0^{(s)}(A_1) = \left[\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3} \right]$$

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

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

$$\boxed{\text{y7}} \quad \mathbb{T}_{1,1}^{(s)}(E) = \left[\frac{\sqrt{2}i}{2}, 0, -\frac{\sqrt{2}i}{2} \right]$$

$$\boxed{\text{y8}} \quad \mathbb{T}_{1,2}^{(s)}(E) = \left[-\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{3}, -\frac{\sqrt{6}i}{6} \right]$$

Table 5: Orbital of each site

| # | site | orbital |
|---|------|--------------------------------------------------------------------------------------------------|
| 1 | A | $ p_x, \uparrow\rangle, p_x, \downarrow\rangle, p_y, \uparrow\rangle, p_y, \downarrow\rangle$ |
| 2 | B | $ p_x, \uparrow\rangle, p_x, \downarrow\rangle, p_y, \uparrow\rangle, p_y, \downarrow\rangle$ |

Table 6: Neighbor and bra-ket of each bond

| # | head | tail | neighbor | head (bra) | tail (ket) |
|---|------|------|----------|------------|------------|
| 1 | A | B | [1] | [p] | [p] |

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

Table 7: 'A' (#1) site cluster (1b), 3m.

| SL | position (\mathbf{s}) | mapping |
|----|------------------------------|---------------|
| 1 | [0.33333, 0.66667, 0.00000] | [1,2,3,4,5,6] |

Table 8: 'B' (#2) site cluster (1c), 3m.

| SL | position (\mathbf{s}) | mapping |
|----|------------------------------|---------------|
| 1 | [0.66667, 0.33333, 0.00000] | [1,2,3,4,5,6] |

Bond in Unit Cell

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

Table 9: 1-th 'A'-'B' [1] (#1) bond cluster (3a@3d), D, $|\mathbf{v}|=0.57735$ (cartesian)

| SL | vector (\mathbf{v}) | center (\mathbf{c}) | mapping | head | tail | \mathbf{R} (primitive) |
|----|------------------------------|------------------------------|---------|-------|-------|--------------------------|
| 1 | [-0.33333, 0.33333, 0.00000] | [0.50000, 0.50000, 0.00000] | [1,4] | (1,1) | (1,1) | [0,0,0] |
| 2 | [-0.33333,-0.66667, 0.00000] | [0.50000, 0.00000, 0.00000] | [2,6] | (1,1) | (1,1) | [0,1,0] |
| 3 | [0.66667, 0.33333, 0.00000] | [0.00000, 0.50000, 0.00000] | [3,5] | (1,1) | (1,1) | [-1,0,0] |

