

Model for “C3v”

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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_1 , A_2 , E]
 - Spin (s): [0, 1]
- Max. neighbor: 10
- Search cell range: (-2, 3), (-2, 3), (-2, 3)
- Toroidal priority: false

Group and Unit Cell

- Group: PG No. 35 $C_{3v}(1)$ $3m$ (31m setting) [trigonal]
- Unit cell:
 $a = 1.00000$, $b = 1.00000$, $c = 10.00000$, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 120.0$
- Lattice vectors (conventional cell):
 $\mathbf{a}_1 = [1.00000, 0.00000, 0.00000]$
 $\mathbf{a}_2 = [-0.50000, 0.86603, 0.00000]$
 $\mathbf{a}_3 = [0.00000, 0.00000, 10.00000]$

Symmetry Operation

Table 1: Symmetry operation

| # | SO | # | SO | # | SO | # | SO | # | SO |
|---|----|---|-------------|---|-------------|---|------------|---|-----------|
| 1 | 1 | 2 | 3_{001}^+ | 3 | 3_{001}^- | 4 | m_{1-10} | 5 | m_{120} |

| | | | | | |
|---|------------------|--|--|--|--|
| 6 | m ₂₁₀ | | | | |
|---|------------------|--|--|--|--|

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 | $\mathbb{Q}_3(A_1, 2)$ | A_1 | 3 | Q, T | 2 | - | $\frac{\sqrt{10}x(x^2-3y^2)}{4}$ |
| 5 | $\mathbb{G}_1(A_2)$ | A_2 | 1 | G, M | - | - | z |
| 6 | $\mathbb{G}_2(A_2)$ | A_2 | 2 | G, M | - | - | $-\frac{x^2}{2} - \frac{y^2}{2} + z^2$ |
| 7 | $\mathbb{Q}_3(A_2)$ | A_2 | 3 | Q, T | - | - | $\frac{\sqrt{10}y(3x^2-y^2)}{4}$ |
| 8 | $\mathbb{Q}_4(A_2)$ | A_2 | 4 | Q, T | - | - | $\frac{\sqrt{70}yz(3x^2-y^2)}{4}$ |
| 9 | $\mathbb{G}_{1,1}(E)$ | E | 1 | G, M | - | 1 | $-y$ |
| 10 | $\mathbb{G}_{1,2}(E)$ | | | | | 2 | x |
| 11 | $\mathbb{Q}_{1,1}(E)$ | E | 1 | Q, T | - | 1 | x |
| 12 | $\mathbb{Q}_{1,2}(E)$ | | | | | 2 | y |
| 13 | $\mathbb{Q}_{2,1}(E, 1)$ | E | 2 | Q, T | 1 | 1 | $\sqrt{3}xz$ |

continued ...

Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|----|--------------------------|--------|------|--------|--------------|-----------|--------------------------------------|
| 14 | $\mathbb{Q}_{2,2}(E, 1)$ | | | | | 2 | $\sqrt{3}yz$ |
| 15 | $\mathbb{Q}_{2,1}(E, 2)$ | E | 2 | Q, T | 2 | 1 | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| 16 | $\mathbb{Q}_{2,2}(E, 2)$ | | | | | 2 | $-\sqrt{3}xy$ |
| 17 | $\mathbb{Q}_{3,1}(E, 1)$ | E | 3 | Q, T | 1 | 1 | $-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$ |
| 18 | $\mathbb{Q}_{3,2}(E, 1)$ | | | | | 2 | $-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$ |
| 19 | $\mathbb{Q}_{3,1}(E, 2)$ | E | 3 | Q, T | 2 | 1 | $-\frac{\sqrt{15}z(x-y)(x+y)}{2}$ |
| 20 | $\mathbb{Q}_{3,2}(E, 2)$ | | | | | 2 | $\sqrt{15}xyz$ |

— Basis in full matrix —

Table 3: dimension = 12

| # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) |
|----|---------------------|----|---------------------|---|---------------------|---|---------------------|----|---------------------|
| 1 | $ s\rangle @A(1)$ | 2 | $ s\rangle @A(2)$ | 3 | $ s\rangle @A(3)$ | 4 | $ p_x\rangle @B(1)$ | 5 | $ p_y\rangle @B(1)$ |
| 6 | $ p_z\rangle @B(1)$ | 7 | $ p_x\rangle @B(2)$ | 8 | $ p_y\rangle @B(2)$ | 9 | $ p_z\rangle @B(2)$ | 10 | $ p_x\rangle @B(3)$ |
| 11 | $ p_y\rangle @B(3)$ | 12 | $ p_z\rangle @B(3)$ | | | | | | |

Table 4: Atomic basis (orbital part only)

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

SAMB

28 (all 42) SAMBs

- 'A' site-cluster

- * bra: $\langle s|$

- * ket: $|s\rangle$

- * wyckoff: **3b**

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

$$\boxed{\text{z15}} \quad \mathbb{Q}_{1,1}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,1}^{(s)}(E)}{2}$$

$$\boxed{\text{z16}} \quad \mathbb{Q}_{1,2}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,2}^{(s)}(E)}{2}$$

- 'B' site-cluster

- * bra: $\langle p_x|, \langle p_y|, \langle p_z|$

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

- * wyckoff: **3b**

$$\boxed{\text{z2}} \quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$$

$$\boxed{\text{z3}} \quad \mathbb{Q}_1^{(c)}(A_1) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 1)\mathbb{Q}_{1,1}^{(s)}(E)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 1)\mathbb{Q}_{1,2}^{(s)}(E)}{2}$$

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

$$\boxed{\text{z5}} \quad \mathbb{Q}_3^{(c)}(A_1, 2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(s)}(E)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(s)}(E)}{2}$$

$$\boxed{\text{z10}} \quad \mathbb{Q}_3^{(c)}(A_2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(s)}(E)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(s)}(E)}{2}$$

$$\boxed{\text{z11}} \quad \mathbb{Q}_{1,1}^{(c)}(E, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,1}^{(s)}(E)}{2}$$

$$\boxed{\text{z17}} \quad \mathbb{Q}_{1,2}^{(c)}(E, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,2}^{(s)}(E)}{2}$$

$$\boxed{\text{z18}} \quad \mathbb{Q}_{1,1}^{(c)}(E, b) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(s)}(E)}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(s)}(E)}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_1)\mathbb{Q}_{1,1}^{(s)}(E)}{14}$$

$$\boxed{\text{z19}} \quad \mathbb{Q}_{1,2}^{(c)}(E, b) = -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(s)}(E)}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(s)}(E)}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_1)\mathbb{Q}_{1,2}^{(s)}(E)}{14}$$

$$\boxed{\text{z20}} \quad \mathbb{Q}_{2,1}^{(c)}(E, 1) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 1)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

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

$$\boxed{\text{z22}} \quad \mathbb{Q}_{2,1}^{(c)}(E, 2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

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

$$\boxed{\text{z24}} \quad \mathbb{Q}_{3,1}^{(c)}(E, 1) = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(s)}(E)}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(s)}(E)}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_1)\mathbb{Q}_{1,1}^{(s)}(E)}{7}$$

$$\boxed{\text{z25}} \quad \mathbb{Q}_{3,2}^{(c)}(E, 1) = -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(s)}(E)}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(s)}(E)}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_1)\mathbb{Q}_{1,2}^{(s)}(E)}{7}$$

$$\boxed{\text{z26}} \quad \mathbb{Q}_{3,1}^{(c)}(E, 2) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E, 1)\mathbb{Q}_{1,1}^{(s)}(E)}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E, 1)\mathbb{Q}_{1,2}^{(s)}(E)}{2}$$

$$\boxed{\text{z27}} \quad \mathbb{Q}_{3,2}^{(c)}(E, 2) = \frac{\mathbb{Q}_{2,1}^{(a)}(E, 1)\mathbb{Q}_{1,2}^{(s)}(E)}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E, 1)\mathbb{Q}_{1,1}^{(s)}(E)}{2}$$

$$\boxed{\text{z28}} \quad \mathbb{G}_2^{(c)}(A_2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 1)\mathbb{Q}_{1,2}^{(s)}(E)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 1)\mathbb{Q}_{1,1}^{(s)}(E)}{2}$$

- 'A'-'A' bond-cluster
 - * bra: $\langle s |$
 - * ket: $|s\rangle$
 - * wyckoff: **3b03b**

$$\boxed{\text{z6}} \quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(b)}(A_1)$$

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

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

- 'A'-'B' bond-cluster
 - * bra: $\langle s |$
 - * ket: $|p_x\rangle, |p_y\rangle, |p_z\rangle$
 - * wyckoff: **6a06c**

$$\boxed{\text{z7}} \quad \mathbb{Q}_0^{(c)}(A_1) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E)\mathbb{Q}_{1,1}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z8}} \quad \mathbb{Q}_1^{(c)}(A_1) = \mathbb{Q}_1^{(a)}(A_1)\mathbb{Q}_0^{(b)}(A_1)$$

$$\boxed{\text{z9}} \quad \mathbb{Q}_3^{(c)}(A_1, 2) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E)\mathbb{Q}_{2,1}^{(b)}(E, 2)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E)\mathbb{Q}_{2,2}^{(b)}(E, 2)}{2}$$

$$\boxed{\text{z12}} \quad \mathbb{Q}_3^{(c)}(A_2) = -\frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E)\mathbb{Q}_{2,2}^{(b)}(E, 2)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E)\mathbb{Q}_{2,1}^{(b)}(E, 2)}{2}$$

$$\boxed{\text{z13}} \quad \mathbb{Q}_4^{(c)}(A_2) = \mathbb{Q}_1^{(a)}(A_1)\mathbb{Q}_3^{(b)}(A_2)$$

$$\boxed{\text{z14}} \quad \mathbb{Q}_{1,1}^{(c)}(E, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E)\mathbb{Q}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z31}} \quad \mathbb{Q}_{1,2}^{(c)}(E, a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E)\mathbb{Q}_0^{(b)}(A_1)}{2}$$

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

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

$$\boxed{\text{z34}} \quad \mathbb{Q}_{2,1}^{(c)}(E, 1) = \frac{\sqrt{2}\mathbb{Q}_1^{(a)}(A_1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z35}} \quad \mathbb{Q}_{2,2}^{(c)}(E, 1) = \frac{\sqrt{2}\mathbb{Q}_1^{(a)}(A_1)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z36}} \quad \mathbb{Q}_{2,1}^{(c)}(E, 2a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E)\mathbb{Q}_3^{(b)}(A_2)}{2}$$

$$\boxed{\text{z37}} \quad \mathbb{Q}_{2,2}^{(c)}(E, 2a) = -\frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E)\mathbb{Q}_3^{(b)}(A_2)}{2}$$

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

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

$$\boxed{\text{z40}} \quad \mathbb{Q}_{3,1}^{(c)}(E, 2) = -\frac{\sqrt{2}\mathbb{Q}_1^{(a)}(A_1)\mathbb{Q}_{2,1}^{(b)}(E, 2)}{2}$$

$$\boxed{\text{z41}} \quad \mathbb{Q}_{3,2}^{(c)}(E, 2) = -\frac{\sqrt{2}\mathbb{Q}_1^{(a)}(A_1)\mathbb{Q}_{2,2}^{(b)}(E, 2)}{2}$$

$$\boxed{\text{z42}} \quad \mathbb{G}_1^{(c)}(A_2) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E)\mathbb{Q}_{1,2}^{(b)}(E)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

- bra: $\langle s|$
- ket: $|s\rangle$

$$\boxed{\text{x1}} \quad \mathbb{Q}_0^{(a)}(A_1) = [1]$$

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

$$\boxed{\text{x2}} \quad \mathbb{Q}_0^{(a)}(A_1) = \begin{bmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$$

$$\boxed{\text{x3}} \quad \mathbb{Q}_2^{(a)}(A_1) = \begin{bmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{bmatrix}$$

$$\boxed{\text{x4}} \quad \mathbb{Q}_{2,1}^{(a)}(E, 1) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{\text{x7}} \quad \mathbb{Q}_{2,2}^{(a)}(E, 2) = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{2} & 0 \\ -\frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x8}} \quad \mathbb{M}_1^{(a)}(A_2) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x9}} \quad \mathbb{M}_{1,1}^{(a)}(E) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \end{bmatrix}$$

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

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

$$\boxed{\text{x11}} \quad \mathbb{Q}_1^{(a)}(A_1) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$$

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

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

$$\boxed{\text{x14}} \quad \mathbb{T}_1^{(a)}(A_1) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{2} \end{bmatrix}$$

$$\boxed{\text{x15}} \quad \mathbb{T}_{1,1}^{(a)}(E) = \begin{bmatrix} \frac{\sqrt{2}i}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x16}} \quad \mathbb{T}_{1,2}^{(a)}(E) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$$

Cluster SAMB

- Site cluster

** Wyckoff: 3b

$$\boxed{\text{y1}} \quad \mathbb{Q}_0^{(s)}(A_1) = \left[\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3} \right]$$

$$\boxed{\text{y2}} \quad \mathbb{Q}_{1,1}^{(s)}(E) = \left[\frac{\sqrt{6}}{3}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y3}} \quad \mathbb{Q}_{1,2}^{(s)}(E) = \left[0, \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

- Bond cluster

** Wyckoff: 3b@3b

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

$$\boxed{\text{y5}} \quad \mathbb{M}_1^{(s)}(A_2) = \left[\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3} \right]$$

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

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

$$\boxed{\text{y8}} \quad \mathbb{T}_{1,1}^{(s)}(E) = \left[0, -\frac{\sqrt{2}i}{2}, \frac{\sqrt{2}i}{2} \right]$$

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

** Wyckoff: 6a@6c

$$\boxed{\text{y10}} \quad \mathbb{Q}_0^{(s)}(A_1) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y11}} \quad \mathbb{T}_0^{(s)}(A_1) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y12}} \quad \mathbb{M}_1^{(s)}(A_2) = \left[\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y13}} \quad \mathbb{Q}_3^{(s)}(A_2) = \left[\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y14}} \quad \mathbb{Q}_{1,1}^{(s)}(E) = \left[\frac{5\sqrt{21}}{42}, -\frac{2\sqrt{21}}{21}, -\frac{\sqrt{21}}{42}, -\frac{\sqrt{21}}{42}, \frac{5\sqrt{21}}{42}, -\frac{2\sqrt{21}}{21} \right]$$

$$\boxed{\text{y15}} \quad \mathbb{Q}_{1,2}^{(s)}(E) = \left[\frac{\sqrt{7}}{14}, \frac{\sqrt{7}}{7}, -\frac{3\sqrt{7}}{14}, \frac{3\sqrt{7}}{14}, -\frac{\sqrt{7}}{14}, -\frac{\sqrt{7}}{7} \right]$$

$$\boxed{\text{y16}} \quad \mathbb{T}_{1,1}^{(s)}(E, a) = \left[\frac{5\sqrt{21}i}{42}, -\frac{2\sqrt{21}i}{21}, -\frac{\sqrt{21}i}{42}, -\frac{\sqrt{21}i}{42}, \frac{5\sqrt{21}i}{42}, -\frac{2\sqrt{21}i}{21} \right]$$

$$\boxed{\text{y17}} \quad \mathbb{T}_{1,2}^{(s)}(E, a) = \left[\frac{\sqrt{7}i}{14}, \frac{\sqrt{7}i}{7}, -\frac{3\sqrt{7}i}{14}, \frac{3\sqrt{7}i}{14}, -\frac{\sqrt{7}i}{14}, -\frac{\sqrt{7}i}{7} \right]$$

$$\boxed{\text{y18}} \quad \mathbb{T}_{1,1}^{(s)}(E, b) = \left[\frac{\sqrt{7}i}{14}, \frac{\sqrt{7}i}{7}, -\frac{3\sqrt{7}i}{14}, -\frac{3\sqrt{7}i}{14}, \frac{\sqrt{7}i}{14}, \frac{\sqrt{7}i}{7} \right]$$

$$\boxed{\text{y19}} \quad \mathbb{T}_{1,2}^{(s)}(E, b) = \left[-\frac{5\sqrt{21}i}{42}, \frac{2\sqrt{21}i}{21}, \frac{\sqrt{21}i}{42}, -\frac{\sqrt{21}i}{42}, \frac{5\sqrt{21}i}{42}, -\frac{2\sqrt{21}i}{21} \right]$$

$$\boxed{\text{y20}} \quad \mathbb{Q}_{2,1}^{(s)}(E, 2) = \left[\frac{\sqrt{7}}{14}, \frac{\sqrt{7}}{7}, -\frac{3\sqrt{7}}{14}, -\frac{3\sqrt{7}}{14}, \frac{\sqrt{7}}{14}, \frac{\sqrt{7}}{7} \right]$$

$$\boxed{\text{y21}} \quad \mathbb{Q}_{2,2}^{(s)}(E, 2) = \left[-\frac{5\sqrt{21}}{42}, \frac{2\sqrt{21}}{21}, \frac{\sqrt{21}}{42}, -\frac{\sqrt{21}}{42}, \frac{5\sqrt{21}}{42}, -\frac{2\sqrt{21}}{21} \right]$$

— Site and Bond —

Table 5: Orbital of each site

| # | site | orbital |
|---|----------|---|
| 1 | A | $ s\rangle$ |
| 2 | B | $ p_x\rangle, p_y\rangle, p_z\rangle$ |

Table 6: Neighbor and bra-ket of each bond

| # | head | tail | neighbor | head (bra) | tail (ket) |
|---|------|------|----------|------------|------------|
| 1 | A | A | [1] | [s] | [s] |
| 2 | A | B | [1] | [s] | [p] |

Site in Unit Cell

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

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

| SL | position (\mathbf{s}) | mapping |
|----|------------------------------|---------|
| 1 | [0.16667, 0.00000, 0.00000] | [1,5] |
| 2 | [0.00000, 0.16667, 0.00000] | [2,4] |
| 3 | [-0.16667,-0.16667, 0.00000] | [3,6] |

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

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

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'-'A' [1] (#1) bond cluster (3b@3b), ND, $|\mathbf{v}| = 0.28868$ (cartesian)

| SL | vector (\mathbf{v}) | center (\mathbf{c}) | mapping | head | tail | \mathbf{R} (primitive) |
|----|------------------------------|------------------------------|---------|-------|-------|--------------------------|
| 1 | [-0.16667,-0.33333, 0.00000] | [-0.08333, 0.00000, 0.00000] | [1,-5] | (3,1) | (2,1) | [0,0,0] |
| 2 | [0.33333, 0.16667, 0.00000] | [0.00000,-0.08333, 0.00000] | [2,-4] | (1,1) | (3,1) | [0,0,0] |
| 3 | [-0.16667, 0.16667, 0.00000] | [0.08333, 0.08333, 0.00000] | [3,-6] | (2,1) | (1,1) | [0,0,0] |

Table 10: 1-th 'A'-'B' [1] (#2) bond cluster (6a06c), D, $|\mathbf{v}|=0.60093$ (cartesian)

| SL | vector (\mathbf{v}) | center (\mathbf{c}) | mapping | head | tail | \mathbf{R} (primitive) |
|----|------------------------------|------------------------------|---------|-------|-------|--------------------------|
| 1 | [0.66667, 0.16667, 0.00000] | [-0.33333, 0.08333, 0.00000] | [1] | (2,1) | (1,1) | [0,0,0] |
| 2 | [-0.16667, 0.50000, 0.00000] | [-0.08333,-0.41667, 0.00000] | [2] | (3,1) | (2,1) | [0,0,0] |
| 3 | [-0.50000,-0.66667, 0.00000] | [0.41667, 0.33333, 0.00000] | [3] | (1,1) | (3,1) | [0,0,0] |
| 4 | [0.16667, 0.66667, 0.00000] | [0.08333,-0.33333, 0.00000] | [4] | (1,1) | (2,1) | [0,0,0] |
| 5 | [0.50000,-0.16667, 0.00000] | [-0.41667,-0.08333, 0.00000] | [5] | (3,1) | (1,1) | [0,0,0] |
| 6 | [-0.66667,-0.50000, 0.00000] | [0.33333, 0.41667, 0.00000] | [6] | (2,1) | (3,1) | [0,0,0] |