# Model for "C3v"

## General Condition

- Basis type: `lg`
- 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: 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):
    $\boldsymbol{a}_1 = $ `[ 1.00000, 0.00000, 0.00000]`
    $\boldsymbol{a}_2 = $ `[-0.50000, 0.86603, 0.00000]`
    $\boldsymbol{a}_3 = $ `[ 0.00000, 0.00000,10.00000]`

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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 | $m_{210}$ | | | | | | | | |

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 | $Q$, $T$ | - | - | $\frac{\sqrt{70}yz(3x^2-y^2)}{4}$ |

*continued ...*

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Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|---|--------|--------|------|---|--------------|-----------|----------|
| 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 | $\sqrt{3}xz$ |
| 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**

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Table 3: dimension = 12

| # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) |
|---|---|---|---|---|---|---|---|---|---|
| 0 | $\lvert s \rangle$ @A(1) | 1 | $\lvert s \rangle$ @A(2) | 2 | $\lvert s \rangle$ @A(3) | 3 | $\lvert p_x \rangle$ @B(1) | 4 | $\lvert p_y \rangle$ @B(1) |
| 5 | $\lvert p_z \rangle$ @B(1) | 6 | $\lvert p_x \rangle$ @B(2) | 7 | $\lvert p_y \rangle$ @B(2) | 8 | $\lvert p_z \rangle$ @B(2) | 9 | $\lvert p_x \rangle$ @B(3) |
| 10 | $\lvert p_y \rangle$ @B(3) | 11 | $\lvert p_z \rangle$ @B(3) | | | | | | |

Table 4: Atomic basis (orbital part only)

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

**———  SAMB  ———————————————————————————————————**

28 (all 42) SAMBs

- 'A' site-cluster
  * bra: $\langle s \rvert$
  * ket: $\lvert s \rangle$
  * wyckoff: 3b

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

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

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

- '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`

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

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

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

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

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

$\boxed{\text{z11}}$ $\quad \mathbb{G}_2^{(c)}(A_2) = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E,1)\mathbb{Q}_{1,2}^{(s)}(E)}{2} - \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E,1)\mathbb{Q}_{1,1}^{(s)}(E)}{2}$

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

$\boxed{\text{z18}}$ $\quad \mathbb{Q}_{1,2}^{(c)}(E,a) = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,2}^{(s)}(E)}{2}$

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

$\boxed{\text{z20}}$ $\quad \mathbb{Q}_{1,2}^{(c)}(E,b) = -\dfrac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_{1,2}^{(s)}(E)}{14} - \dfrac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_{1,1}^{(s)}(E)}{14} - \dfrac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_1)\mathbb{Q}_{1,2}^{(s)}(E)}{14}$

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

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

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

$\boxed{\text{z24}}$  $\mathbb{Q}_{2,2}^{(c)}(E,2) = \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_0^{(s)}(A_1)}{2}$

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

$\boxed{\text{z26}}$  $\mathbb{Q}_{3,2}^{(c)}(E,1) = -\dfrac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_{1,2}^{(s)}(E)}{14} - \dfrac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_{1,1}^{(s)}(E)}{14} + \dfrac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_1)\mathbb{Q}_{1,2}^{(s)}(E)}{7}$

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

$\boxed{\text{z28}}$  $\mathbb{Q}_{3,2}^{(c)}(E,2) = \dfrac{\mathbb{Q}_{2,1}^{(a)}(E,1)\mathbb{Q}_{1,2}^{(s)}(E)}{2} + \dfrac{\mathbb{Q}_{2,2}^{(a)}(E,1)\mathbb{Q}_{1,1}^{(s)}(E)}{2}$

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

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

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

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

- 'A'-'B' bond-cluster
  * bra: $\langle s|$

* ket: $|p_x\rangle$, $|p_y\rangle$, $|p_z\rangle$
* wyckoff: `6a@6c`

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

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

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

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

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

$\boxed{\text{z14}}$ $\quad \mathbb{G}_1^{(c)}(A_2) = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E)\mathbb{Q}_{1,2}^{(b)}(E)}{2} - \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$

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

$\boxed{\text{z32}}$ $\quad \mathbb{Q}_{1,2}^{(c)}(E,a) = \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E)\mathbb{Q}_0^{(b)}(A_1)}{2}$

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

$\boxed{\text{z34}}$ $\quad \mathbb{Q}_{1,2}^{(c)}(E,b) = -\dfrac{\mathbb{Q}_{1,1}^{(a)}(E)\mathbb{Q}_{2,2}^{(b)}(E,2)}{2} - \dfrac{\mathbb{Q}_{1,2}^{(a)}(E)\mathbb{Q}_{2,1}^{(b)}(E,2)}{2}$

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

$\boxed{\text{z36}}$ $\quad \mathbb{Q}_{2,2}^{(c)}(E,1) = \dfrac{\sqrt{2}\mathbb{Q}_1^{(a)}(A_1)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$

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

$\boxed{\text{z38}}$  $\mathbb{Q}_{2,2}^{(c)}(E, 2a) = -\dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E)\mathbb{Q}_3^{(b)}(A_2)}{2}$

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

$\boxed{\text{z40}}$  $\mathbb{Q}_{2,2}^{(c)}(E, 2b) = -\dfrac{\mathbb{Q}_{1,1}^{(a)}(E)\mathbb{Q}_{1,2}^{(b)}(E)}{2} - \dfrac{\mathbb{Q}_{1,2}^{(a)}(E)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$

$\boxed{\text{z41}}$  $\mathbb{Q}_{3,1}^{(c)}(E, 2) = -\dfrac{\sqrt{2}\mathbb{Q}_1^{(a)}(A_1)\mathbb{Q}_{2,1}^{(b)}(E, 2)}{2}$

$\boxed{\text{z42}}$  $\mathbb{Q}_{3,2}^{(c)}(E, 2) = -\dfrac{\sqrt{2}\mathbb{Q}_1^{(a)}(A_1)\mathbb{Q}_{2,2}^{(b)}(E, 2)}{2}$

—— **Atomic SAMB** ————————————————————————————————————

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

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

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

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

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

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

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

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

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

$\boxed{\text{x8}}$ $\mathbb{M}_{1}^{(a)}(A_2) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$

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

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

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

$\boxed{\text{x11}}$ $\mathbb{Q}_{1}^{(a)}(A_1) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$

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

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

$\boxed{\text{x14}}$ $\mathbb{T}_{1}^{(a)}(A_1) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{2} \end{bmatrix}$

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

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

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- Site cluster

** Wyckoff: `3b`

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

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

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

- Bond cluster

** Wyckoff: `3b@3b`

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

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

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

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

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

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

** Wyckoff: `6a@6c`

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

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

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

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

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

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

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

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

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

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

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

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

— **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 ($s$) | mapping |
|----|----------------|---------|
| 1 | [ 0.16667, 0.00000, 0.00000] | [1,5] |

*continued …*

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Table 7

| SL | position ($s$) | mapping |
|----|----------------|---------|
| 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 ($s$) | 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, $|v|= 0.28868$ (cartesian)

| SL | vector $(v)$ | center $(c)$ | mapping | head | tail | $R$ (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 (`6a@6c`), D, $|v|= 0.60093$ (cartesian)

| SL | vector $(v)$ | center $(c)$ | mapping | head | tail | $R$ (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] |