Model for "C3v"

Generated on 2026-01-18 16:52:48 by MultiPie 2.0.0

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]`
- 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]

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	-	$\frac{\sqrt{10}x\left(x^2-3y^2\right)}{4}$
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	-	-	$\frac{\sqrt{10}y\left(3x^2-y^2\right)}{4}$
8	$\mathbb{Q}_4(A_2)$	A_2	4	Q, T	-	-	$\frac{\sqrt{70}yz\left(3x^2-y^2\right)}{4}$
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	$-\frac{\sqrt{6}x\left(x^2+y^2-4z^2\right)}{4}$
18	$\mathbb{Q}_{3,2}(E,1)$					2	$-\frac{\sqrt{6}y\left(x^2+y^2-4z^2\right)}{4}$
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	$\lvert s\rangle$ @A(1)	2	$\lvert s\rangle$ @A(2)	3	$\lvert s\rangle$ @A(3)	4	$\lvert p_x\rangle$ @B(1)	5	$\lvert p_y\rangle$ @B(1)
6	$\lvert p_z\rangle$ @B(1)	7	$\lvert p_x\rangle$ @B(2)	8	$\lvert p_y\rangle$ @B(2)	9	$\lvert p_z\rangle$ @B(2)	10	$\lvert p_x\rangle$ @B(3)
11	$\lvert p_y\rangle$ @B(3)	12	$\lvert p_z\rangle$ @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`

$\boxed{\text{z1}}$ $\mathbb{Q}_{0}^{(c)}(A_1) = \mathbb{Q}_{0}^{(a)}(A_1)\mathbb{Q}_{0}^{(s)}(A_1)$

$\boxed{\text{z15}}$ $\mathbb{Q}_{1,1}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A_1)\mathbb{Q}_{1,1}^{(s)}(E)}{2}$

$\boxed{\text{z16}}$ $\mathbb{Q}_{1,2}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A_1)\mathbb{Q}_{1,2}^{(s)}(E)}{2}$

- 'B' site-cluster
  * bra: $\langle p_x\rvert$, $\langle p_y\rvert$, $\langle p_z\rvert$
  * ket: $\lvert p_x\rangle$, $\lvert p_y\rangle$, $\lvert p_z\rangle$
  * wyckoff: `3b`

$\boxed{\text{z2}}$ $\mathbb{Q}_{0}^{(c)}(A_1) = \mathbb{Q}_{0}^{(a)}(A_1)\mathbb{Q}_{0}^{(s)}(A_1)$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$\boxed{\text{z6}}$ $$\mathbb{Q}_{0}^{(c)}(A_1) = \mathbb{Q}_{0}^{(a)}(A_1)\mathbb{Q}_{0}^{(b)}(A_1)$$

$\boxed{\text{z29}}$ $$\mathbb{Q}_{1,1}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A_1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$\boxed{\text{z30}}$ $$\mathbb{Q}_{1,2}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A_1)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

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

$\boxed{\text{z7}}$ $$\mathbb{Q}_{0}^{(c)}(A_1) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E)\mathbb{Q}_{1,1}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$\boxed{\text{z8}}$ $$\mathbb{Q}_{1}^{(c)}(A_1) = \mathbb{Q}_{1}^{(a)}(A_1)\mathbb{Q}_{0}^{(b)}(A_1)$$

$\boxed{\text{z9}}$ $$\mathbb{Q}_{3}^{(c)}(A_1,2) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E)\mathbb{Q}_{2,1}^{(b)}(E,2)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E)\mathbb{Q}_{2,2}^{(b)}(E,2)}{2}$$

$\boxed{\text{z12}}$ $$\mathbb{Q}_{3}^{(c)}(A_2) = -\frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E)\mathbb{Q}_{2,2}^{(b)}(E,2)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E)\mathbb{Q}_{2,1}^{(b)}(E,2)}{2}$$

$\boxed{\text{z13}}$ $$\mathbb{Q}_{4}^{(c)}(A_2) = \mathbb{Q}_{1}^{(a)}(A_1)\mathbb{Q}_{3}^{(b)}(A_2)$$

$\boxed{\text{z14}}$ $\mathbb{Q}^{(c)}_{1,1}(E,a) = \frac{\sqrt{2}\mathbb{Q}^{(a)}_{1,1}(E)\mathbb{Q}^{(b)}_{0}(A_1)}{2}$

$\boxed{\text{z31}}$ $\mathbb{Q}^{(c)}_{1,2}(E,a) = \frac{\sqrt{2}\mathbb{Q}^{(a)}_{1,2}(E)\mathbb{Q}^{(b)}_{0}(A_1)}{2}$

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

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

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

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

$\boxed{\text{z36}}$ $\mathbb{Q}^{(c)}_{2,1}(E,2a) = \frac{\sqrt{2}\mathbb{Q}^{(a)}_{1,2}(E)\mathbb{Q}^{(b)}_{3}(A_2)}{2}$

$\boxed{\text{z37}}$ $\mathbb{Q}^{(c)}_{2,2}(E,2a) = -\frac{\sqrt{2}\mathbb{Q}^{(a)}_{1,1}(E)\mathbb{Q}^{(b)}_{3}(A_2)}{2}$

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

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

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

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

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

Atomic SAMB

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

— Cluster SAMB

- Site cluster

** Wyckoff: `3b`

$\boxed{\text{y1}}$ $\mathbb{Q}_{0}^{(s)}(A_1) = \left[\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}\right]$

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

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

- Bond cluster

** Wyckoff: `3b@3b`

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

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

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

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

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

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

** Wyckoff: `6a@6c`

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

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

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

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

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

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

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

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

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

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

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

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

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 ($\boldsymbol{s}$)	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 ($\boldsymbol{s}$)	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, $|\boldsymbol{v}|$= 0.28868 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (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, $|\boldsymbol{v}|$= 0.60093 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (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]