

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.: **[A₁, A₂, 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.: **[A₁, A₂, E]**
 - Spin (s): **[0, 1]**
- Site-cluster selection:
 - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
 - Irrep.: **[A₁, A₂, E]**
- Bond-cluster selection:
 - Type: **[Q, G, M, T]**
 - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
 - Irrep.: **[A₁, A₂, 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):
 - $\mathbf{a}_1 = [1.00000, 0.00000, 0.00000]$
 - $\mathbf{a}_2 = [-0.50000, 0.86603, 0.00000]$
 - $\mathbf{a}_3 = [0.00000, 0.00000, 10.00000]$

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	$Q_0(A_1)$	A_1	0	Q, T	-	-	1
2	$Q_1(A_1)$	A_1	1	Q, T	-	-	z
3	$Q_2(A_1)$	A_1	2	Q, T	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
4	$Q_3(A_1, 2)$	A_1	3	Q, T	2	-	$\frac{\sqrt{10}x(x^2-3y^2)}{4}$
5	$G_1(A_2)$	A_2	1	G, M	-	-	z
6	$G_2(A_2)$	A_2	2	G, M	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
7	$Q_3(A_2)$	A_2	3	Q, T	-	-	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$
8	$Q_4(A_2)$	A_2	4	Q, T	-	-	$\frac{\sqrt{70}yz(3x^2-y^2)}{4}$

continued ...

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 —

Table 3: dimension = 12

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

42 (all 42) SAMBs

- 'A' site-cluster : **A**
 - * 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 : B

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

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

* wyckoff: 3b

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

• 'A'-'A' bond-cluster : A;A_001_1

* 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 : B;A_001_1

* bra: $\langle s |$

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

* wyckoff: **6a06c**

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Atomic SAMB

- 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

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

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

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

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

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

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

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

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

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

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

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

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

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]

continued ...

Table 7

SL	position (\mathbf{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 (\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 (3b03b), 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]