

# 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<sub>1</sub>, A<sub>2</sub>, 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<sub>1</sub>, A<sub>2</sub>, E]**
  - Spin (s): **[0, 1]**
- Site-cluster selection:
  - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
  - Irrep.: **[A<sub>1</sub>, A<sub>2</sub>, E]**
- Bond-cluster selection:
  - Type: **[Q, G, M, T]**
  - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
  - Irrep.: **[A<sub>1</sub>, A<sub>2</sub>, E]**
- Max. neighbor: **10**
- Search cell range: **(-2, 3), (-2, 3), (-2, 3)**
- Toroidal priority: **false**

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## 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):
  - $\mathbf{a}_1 = [ 1.00000, 0.00000, 0.00000 ]$
  - $\mathbf{a}_2 = [ -0.50000, 0.86603, 0.00000 ]$
  - $\mathbf{a}_3 = [ 0.00000, 0.00000, 10.00000 ]$

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## Symmetry Operation

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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	$m_{210}$								

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## Harmonics

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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	$-y$

*continued ...*

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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	$\sqrt{15}xyz$

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**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	$ 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$	$z$

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— SAMB: 42 (all 42)

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• A : '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 : '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**

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

• **A;A\_001\_1** : 'A'-'A' bond-cluster

\* bra:  $\langle s |$

\* ket:  $|s\rangle$

\* wyckoff: **3b@3b**

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

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

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

• **B;A\_001\_1** : 'A'-'B' bond-cluster

\* bra:  $\langle s |$

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

\* wyckoff: **6a@6c**

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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## Cluster SAMB

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- 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 ( $s$ )	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 (6a@6c), 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]

*continued ...*

Table 10

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