

Model for “Te”

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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]**
- 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: SG No. 152 D_3^4 $P3_121$ [trigonal]
- Associated point group: PG No. 152 D_3 32 (321 setting) [trigonal]
- Unit cell:
 - $a = 4.45800$, $b = 4.45800$, $c = 5.92500$, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 120.0$
- Lattice vectors (conventional cell):
 - $\mathbf{a}_1 = [4.45800, 0.00000, 0.00000]$
 - $\mathbf{a}_2 = [-2.22900, 3.86074, 0.00000]$
 - $\mathbf{a}_3 = [0.00000, 0.00000, 5.92500]$

Symmetry Operation

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	$\{1 0\}$	2	$\{3_{001}^+ 00\frac{1}{3}\}$	3	$\{3_{001}^- 00\frac{2}{3}\}$	4	$\{2_{110} 0\}$	5	$\{2_{100} 00\frac{2}{3}\}$
6	$\{2_{010} 00\frac{1}{3}\}$								

Harmonics

Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$G_0(A_1)$	A_1	0	G, M	-	-	1
2	$Q_0(A_1)$	A_1	0	Q, T	-	-	1
3	$G_2(A_1)$	A_1	2	G, M	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
4	$Q_2(A_1)$	A_1	2	Q, T	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
5	$Q_3(A_1)$	A_1	3	Q, T	-	-	$\frac{\sqrt{10}x(x^2-3y^2)}{4}$
6	$G_1(A_2)$	A_2	1	G, M	-	-	z
7	$Q_1(A_2)$	A_2	1	Q, T	-	-	z
8	$Q_3(A_2, 2)$	A_2	3	Q, T	2	-	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
9	$\mathbb{G}_{1,1}(E)$	E	1	G, M	-	1	x
10	$\mathbb{G}_{1,2}(E)$					2	y
11	$\mathbb{Q}_{1,1}(E)$	E	1	Q, T	-	1	x
12	$\mathbb{Q}_{1,2}(E)$					2	y
13	$\mathbb{G}_{2,1}(E, 1)$	E	2	G, M	1	1	$\sqrt{3}yz$
14	$\mathbb{G}_{2,2}(E, 1)$					2	$-\sqrt{3}xz$
15	$\mathbb{G}_{2,1}(E, 2)$	E	2	G, M	2	1	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
16	$\mathbb{G}_{2,2}(E, 2)$					2	$-\sqrt{3}xy$
17	$\mathbb{Q}_{2,1}(E, 1)$	E	2	Q, T	1	1	$\sqrt{3}yz$
18	$\mathbb{Q}_{2,2}(E, 1)$					2	$-\sqrt{3}xz$
19	$\mathbb{Q}_{2,1}(E, 2)$	E	2	Q, T	2	1	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
20	$\mathbb{Q}_{2,2}(E, 2)$					2	$-\sqrt{3}xy$
21	$\mathbb{Q}_{3,1}(E, 1)$	E	3	Q, T	1	1	$-\frac{\sqrt{6}x(x^2+y^2-4z^2)}{4}$
22	$\mathbb{Q}_{3,2}(E, 1)$					2	$-\frac{\sqrt{6}y(x^2+y^2-4z^2)}{4}$
23	$\mathbb{Q}_{3,1}(E, 2)$	E	3	Q, T	2	1	$\sqrt{15}xyz$
24	$\mathbb{Q}_{3,2}(E, 2)$					2	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$

Basis in full matrix

Table 3: dimension = 9

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

Table 4: Atomic basis (orbital part only)

orbital	definition
$ p_x\rangle$	x
$ p_y\rangle$	y
$ p_z\rangle$	z

SAMB

30 (all 45) SAMBs

• 'A' site-cluster

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

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

* wyckoff: **3a**

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

$$\boxed{\text{z2}} \quad \mathbb{Q}_2^{(c)}(A_1) = \mathbb{Q}_2^{(a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$$

$$\boxed{\text{z3}} \quad \mathbb{Q}_3^{(c)}(A_1) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(s)}(E)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(s)}(E)}{2}$$

$$\boxed{\text{z4}} \quad \mathbb{G}_2^{(c)}(A_1) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 1)\mathbb{Q}_{1,1}^{(s)}(E)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 1)\mathbb{Q}_{1,2}^{(s)}(E)}{2}$$

$$\boxed{\text{z11}} \quad \mathbb{Q}_1^{(c)}(A_2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 1)\mathbb{Q}_{1,2}^{(s)}(E)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 1)\mathbb{Q}_{1,1}^{(s)}(E)}{2}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

• 'A'-'A' bond-cluster

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

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

* wyckoff: **3a@3b**

$$\boxed{\text{z5}} \quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(b)}(A_1)$$

$$\boxed{\text{z6}} \quad \mathbb{Q}_2^{(c)}(A_1) = \mathbb{Q}_2^{(a)}(A_1)\mathbb{Q}_0^{(b)}(A_1)$$

$$\boxed{\text{z7}} \quad \mathbb{Q}_3^{(c)}(A_1) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z8}} \quad \mathbb{G}_0^{(c)}(A_1) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{3} + \frac{\sqrt{3}\mathbb{M}_1^{(a)}(A_2)\mathbb{T}_1^{(b)}(A_2)}{3}$$

$$\boxed{\text{z9}} \quad \mathbb{G}_2^{(c)}(A_1, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 1)\mathbb{Q}_{1,1}^{(b)}(E)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 1)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z10}} \quad \mathbb{G}_2^{(c)}(A_1, b) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{6} + \frac{\sqrt{6}\mathbb{M}_1^{(a)}(A_2)\mathbb{T}_1^{(b)}(A_2)}{3}$$

$$\boxed{\text{z13}} \quad \mathbb{Q}_1^{(c)}(A_2, a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 1)\mathbb{Q}_{1,2}^{(b)}(E)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

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

$$\boxed{\text{z15}} \quad \mathbb{Q}_3^{(c)}(A_2, 2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(b)}(E)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z28}} \quad \mathbb{Q}_{1,1}^{(c)}(E, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$$\begin{aligned}
\boxed{\text{z29}} \quad \mathbb{Q}_{1,2}^{(c)}(E, a) &= \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,2}^{(b)}(E)}{2} \\
\boxed{\text{z30}} \quad \mathbb{Q}_{1,1}^{(c)}(E, b) &= \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(b)}(E)}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(b)}(E)}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_1)\mathbb{Q}_{1,1}^{(b)}(E)}{14} \\
\boxed{\text{z31}} \quad \mathbb{Q}_{1,2}^{(c)}(E, b) &= -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(b)}(E)}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(b)}(E)}{14} - \frac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_1)\mathbb{Q}_{1,2}^{(b)}(E)}{14} \\
\boxed{\text{z32}} \quad \mathbb{Q}_{1,1}^{(c)}(E, c) &= \frac{\mathbb{M}_{1,2}^{(a)}(E)\mathbb{T}_1^{(b)}(A_2)}{2} - \frac{\mathbb{M}_1^{(a)}(A_2)\mathbb{T}_{1,2}^{(b)}(E)}{2} \\
\boxed{\text{z33}} \quad \mathbb{Q}_{1,2}^{(c)}(E, c) &= -\frac{\mathbb{M}_{1,1}^{(a)}(E)\mathbb{T}_1^{(b)}(A_2)}{2} + \frac{\mathbb{M}_1^{(a)}(A_2)\mathbb{T}_{1,1}^{(b)}(E)}{2} \\
\boxed{\text{z34}} \quad \mathbb{Q}_{2,1}^{(c)}(E, 1) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 1)\mathbb{Q}_0^{(b)}(A_1)}{2} \\
\boxed{\text{z35}} \quad \mathbb{Q}_{2,2}^{(c)}(E, 1) &= \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 1)\mathbb{Q}_0^{(b)}(A_1)}{2} \\
\boxed{\text{z36}} \quad \mathbb{Q}_{2,1}^{(c)}(E, 2) &= \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_0^{(b)}(A_1)}{2} \\
\boxed{\text{z37}} \quad \mathbb{Q}_{2,2}^{(c)}(E, 2) &= \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_0^{(b)}(A_1)}{2} \\
\boxed{\text{z38}} \quad \mathbb{Q}_{3,1}^{(c)}(E, 1) &= \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(b)}(E)}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(b)}(E)}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_1)\mathbb{Q}_{1,1}^{(b)}(E)}{7} \\
\boxed{\text{z39}} \quad \mathbb{Q}_{3,2}^{(c)}(E, 1) &= -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E, 2)\mathbb{Q}_{1,2}^{(b)}(E)}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E, 2)\mathbb{Q}_{1,1}^{(b)}(E)}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_1)\mathbb{Q}_{1,2}^{(b)}(E)}{7} \\
\boxed{\text{z40}} \quad \mathbb{Q}_{3,1}^{(c)}(E, 2) &= \frac{\mathbb{Q}_{2,1}^{(a)}(E, 1)\mathbb{Q}_{1,1}^{(b)}(E)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E, 1)\mathbb{Q}_{1,2}^{(b)}(E)}{2} \\
\boxed{\text{z41}} \quad \mathbb{Q}_{3,2}^{(c)}(E, 2) &= -\frac{\mathbb{Q}_{2,1}^{(a)}(E, 1)\mathbb{Q}_{1,2}^{(b)}(E)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E, 1)\mathbb{Q}_{1,1}^{(b)}(E)}{2} \\
\boxed{\text{z42}} \quad \mathbb{G}_{2,1}^{(c)}(E, 1) &= \frac{\mathbb{M}_{1,2}^{(a)}(E)\mathbb{T}_1^{(b)}(A_2)}{2} + \frac{\mathbb{M}_1^{(a)}(A_2)\mathbb{T}_{1,2}^{(b)}(E)}{2}
\end{aligned}$$

$$\boxed{\text{z43}} \quad \mathbb{G}_{2,2}^{(c)}(E, 1) = -\frac{\mathbb{M}_{1,1}^{(a)}(E)\mathbb{T}_1^{(b)}(A_2)}{2} - \frac{\mathbb{M}_1^{(a)}(A_2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z44}} \quad \mathbb{G}_{2,1}^{(c)}(E, 2) = \frac{\mathbb{M}_{1,1}^{(a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z45}} \quad \mathbb{G}_{2,2}^{(c)}(E, 2) = -\frac{\mathbb{M}_{1,1}^{(a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

Atomic SAMB

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

$$\boxed{\text{x1}} \quad \mathbb{Q}_0^{(a)}(A_1) = \begin{bmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$$

$$\boxed{\text{x2}} \quad \mathbb{Q}_2^{(a)}(A_1) = \begin{bmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{bmatrix}$$

$$\boxed{\text{x3}} \quad \mathbb{Q}_{2,1}^{(a)}(E, 1) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$$

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

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

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

$$\boxed{\text{x7}} \quad \mathbb{M}_1^{(a)}(A_2) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

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

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

Cluster SAMB

- Site cluster

** Wyckoff: **3a**

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

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

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

- Bond cluster

** Wyckoff: **3a@3b**

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

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

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

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

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

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

Site and Bond

Table 5: Orbital of each site

#	site	orbital
1	A	$ 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]	[p]	[p]

Site in Unit Cell

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

Table 7: 'A' (#1) site cluster (3a), .2.

SL	position (\mathbf{s})	mapping
1	[0.27400, 0.00000, 0.33333]	[1,5]
2	[0.00000, 0.27400, 0.66667]	[2,4]
3	[0.72600, 0.72600, 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 8: 1-th 'A'-'A' [1] (#1) bond cluster (3a@3b), ND, $|\mathbf{v}| = 2.89426$ (cartesian)

SL	vector (\mathbf{v})	center (\mathbf{c})	mapping	head	tail	\mathbf{R} (primitive)
1	[-0.27400, -0.54800, 0.33333]	[0.86300, 0.00000, 0.83333]	[1,-5]	(3,1)	(2,1)	[1,1,-1]
2	[0.54800, 0.27400, 0.33333]	[0.00000, 0.86300, 0.16667]	[2,-4]	(1,1)	(3,1)	[-1,-1,0]
3	[-0.27400, 0.27400, 0.33333]	[0.13700, 0.13700, 0.50000]	[3,-6]	(2,1)	(1,1)	[0,0,0]