Model for “Te”

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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: 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):
  $\boldsymbol{a}_1 =$ `[ 4.45800, 0.00000, 0.00000]`
  $\boldsymbol{a}_2 =$ `[-2.22900, 3.86074, 0.00000]`
  $\boldsymbol{a}_3 =$ `[ 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	$\mathbb{G}_0(A_1)$	A_1	0	G, M	-	-	1
2	$\mathbb{Q}_0(A_1)$	A_1	0	Q, T	-	-	1
3	$\mathbb{G}_2(A_1)$	A_1	2	G, M	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
4	$\mathbb{Q}_2(A_1)$	A_1	2	Q, T	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
5	$\mathbb{Q}_3(A_1)$	A_1	3	Q, T	-	-	$\frac{\sqrt{10}x\left(x^2-3y^2\right)}{4}$
6	$\mathbb{G}_1(A_2)$	A_2	1	G, M	-	-	z
7	$\mathbb{Q}_1(A_2)$	A_2	1	Q, T	-	-	z
8	$\mathbb{Q}_3(A_2, 2)$	A_2	3	Q, T	2	-	$\frac{\sqrt{10}y\left(3x^2-y^2\right)}{4}$

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	$-\frac{\sqrt{6}x\left(x^2+y^2-4z^2\right)}{4}$
22	$\mathbb{Q}_{3,2}(E,1)$					2	$-\frac{\sqrt{6}y\left(x^2+y^2-4z^2\right)}{4}$
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	$\lvert p_x \rangle$ @A(1)	1	$\lvert p_y \rangle$ @A(1)	2	$\lvert p_z \rangle$ @A(1)	3	$\lvert p_x \rangle$ @A(2)	4	$\lvert p_y \rangle$ @A(2)
5	$\lvert p_z \rangle$ @A(2)	6	$\lvert p_x \rangle$ @A(3)	7	$\lvert p_y \rangle$ @A(3)	8	$\lvert p_z \rangle$ @A(3)		

Table 4: Atomic basis (orbital part only)

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

SAMB

45 (all 45) SAMBs

- 'A' site-cluster : `A`
  - * 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: `3a`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 'A'-'A' bond-cluster : `A;A_001_1`
  * bra: $\langle p_x|$, $\langle p_y|$, $\langle p_z|$
  * ket: $|p_x\rangle$, $|p_y\rangle$, $|p_z\rangle$
  * wyckoff: `3a@3b`

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

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

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

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

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

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

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

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

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

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

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

$\boxed{\text{z30}}$ $$\mathbb{Q}^{(c)}_{1,1}(E,b) = \frac{\sqrt{42}\mathbb{Q}^{(a)}_{2,1}(E,2)\mathbb{Q}^{(b)}_{1,1}(E)}{14} - \frac{\sqrt{42}\mathbb{Q}^{(a)}_{2,2}(E,2)\mathbb{Q}^{(b)}_{1,2}(E)}{14} - \frac{\sqrt{14}\mathbb{Q}^{(a)}_{2}(A_1)\mathbb{Q}^{(b)}_{1,1}(E)}{14}$$

$\boxed{\text{z31}}$ $$\mathbb{Q}^{(c)}_{1,2}(E,b) = -\frac{\sqrt{42}\mathbb{Q}^{(a)}_{2,1}(E,2)\mathbb{Q}^{(b)}_{1,2}(E)}{14} - \frac{\sqrt{42}\mathbb{Q}^{(a)}_{2,2}(E,2)\mathbb{Q}^{(b)}_{1,1}(E)}{14} - \frac{\sqrt{14}\mathbb{Q}^{(a)}_{2}(A_1)\mathbb{Q}^{(b)}_{1,2}(E)}{14}$$

$\boxed{\text{z32}}$ $$\mathbb{Q}^{(c)}_{1,1}(E,c) = \frac{\mathbb{M}^{(a)}_{1,2}(E)\mathbb{T}^{(b)}_{1}(A_2)}{2} - \frac{\mathbb{M}^{(a)}_{1}(A_2)\mathbb{T}^{(b)}_{1,2}(E)}{2}$$

$\boxed{\text{z33}}$ $$\mathbb{Q}^{(c)}_{1,2}(E,c) = -\frac{\mathbb{M}^{(a)}_{1,1}(E)\mathbb{T}^{(b)}_{1}(A_2)}{2} + \frac{\mathbb{M}^{(a)}_{1}(A_2)\mathbb{T}^{(b)}_{1,1}(E)}{2}$$

$\boxed{\text{z34}}$ $$\mathbb{Q}^{(c)}_{2,1}(E,1) = \frac{\sqrt{2}\mathbb{Q}^{(a)}_{2,1}(E,1)\mathbb{Q}^{(b)}_{0}(A_1)}{2}$$

$\boxed{\text{z35}}$ $$\mathbb{Q}^{(c)}_{2,2}(E,1) = \frac{\sqrt{2}\mathbb{Q}^{(a)}_{2,2}(E,1)\mathbb{Q}^{(b)}_{0}(A_1)}{2}$$

$\boxed{\text{z36}}$ $$\mathbb{Q}^{(c)}_{2,1}(E,2) = \frac{\sqrt{2}\mathbb{Q}^{(a)}_{2,1}(E,2)\mathbb{Q}^{(b)}_{0}(A_1)}{2}$$

$\boxed{\text{z37}}$ $$\mathbb{Q}^{(c)}_{2,2}(E,2) = \frac{\sqrt{2}\mathbb{Q}^{(a)}_{2,2}(E,2)\mathbb{Q}^{(b)}_{0}(A_1)}{2}$$

$\boxed{\text{z38}}$ $$\mathbb{Q}^{(c)}_{3,1}(E,1) = \frac{\sqrt{7}\mathbb{Q}^{(a)}_{2,1}(E,2)\mathbb{Q}^{(b)}_{1,1}(E)}{14} - \frac{\sqrt{7}\mathbb{Q}^{(a)}_{2,2}(E,2)\mathbb{Q}^{(b)}_{1,2}(E)}{14} + \frac{\sqrt{21}\mathbb{Q}^{(a)}_{2}(A_1)\mathbb{Q}^{(b)}_{1,1}(E)}{7}$$

$\boxed{\text{z39}}$ $$\mathbb{Q}^{(c)}_{3,2}(E,1) = -\frac{\sqrt{7}\mathbb{Q}^{(a)}_{2,1}(E,2)\mathbb{Q}^{(b)}_{1,2}(E)}{14} - \frac{\sqrt{7}\mathbb{Q}^{(a)}_{2,2}(E,2)\mathbb{Q}^{(b)}_{1,1}(E)}{14} + \frac{\sqrt{21}\mathbb{Q}^{(a)}_{2}(A_1)\mathbb{Q}^{(b)}_{1,2}(E)}{7}$$

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

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

$\boxed{\text{z42}}$ $$\mathbb{G}^{(c)}_{2,1}(E,1) = \frac{\mathbb{M}^{(a)}_{1,2}(E)\mathbb{T}^{(b)}_{1}(A_2)}{2} + \frac{\mathbb{M}^{(a)}_{1}(A_2)\mathbb{T}^{(b)}_{1,2}(E)}{2}$$

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

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

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

Atomic SAMB

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

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

x2 $\mathbb{Q}_{2}^{(a)}(A_1) = \begin{bmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{bmatrix}$

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

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

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

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

$\boxed{\text{x7}}$ $\mathbb{M}_{1}^{(a)}(A_2) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$

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

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

Cluster SAMB

- Site cluster

** Wyckoff: `3a`

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

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

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

- Bond cluster

** Wyckoff: `3a@3b`

$\boxed{\text{y4}}$ $\mathbb{Q}_{0}^{(s)}(A_1) = \left[\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}\right]$

$\boxed{\text{y5}}$ $\mathbb{T}_{1}^{(s)}(A_2) = \left[\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}\right]$

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

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

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

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

Site and Bond

Table 5: Orbital of each site

#	site	orbital
1	A	$\lvert p_x\rangle$, $\lvert p_y\rangle$, $\lvert p_z\rangle$

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 ($\boldsymbol{s}$)	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, $|\boldsymbol{v}|$= 2.89426 (cartesian)

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