Model for "Te"

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: 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	$\{2_{100}\|00\frac{2}{3}\}$

continued …

Table 1

#	SO	#	SO	#	SO	#	SO	#	SO
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	-	-	$\frac{\sqrt{10}x(x^2 - 3y^2)}{4}$
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	-	$\frac{\sqrt{10}y(3x^2 - y^2)}{4}$
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

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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)
1	$\lvert p_x \rangle$ @A(1)	2	$\lvert p_y \rangle$ @A(1)	3	$\lvert p_z \rangle$ @A(1)	4	$\lvert p_x \rangle$ @A(2)	5	$\lvert p_y \rangle$ @A(2)
6	$\lvert p_z \rangle$ @A(2)	7	$\lvert p_x \rangle$ @A(3)	8	$\lvert p_y \rangle$ @A(3)	9	$\lvert p_z \rangle$ @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** ---

30 (all 45) SAMBs

- 'A' 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: 3a

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

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

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

$\boxed{\text{z4}}$ $\quad \mathbb{Q}_1^{(c)}(A_2) = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E,1)\mathbb{Q}_{1,2}^{(s)}(E)}{2} - \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E,1)\mathbb{Q}_{1,1}^{(s)}(E)}{2}$

$\boxed{\text{z11}}$ $\quad \mathbb{Q}_3^{(c)}(A_2,2) = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_{1,2}^{(s)}(E)}{2} - \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_{1,1}^{(s)}(E)}{2}$

$\boxed{\text{z12}}$ $\quad \mathbb{Q}_{1,1}^{(c)}(E,a) = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,1}^{(s)}(E)}{2}$

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

$\boxed{\text{z17}}$ $\quad \mathbb{Q}_{1,1}^{(c)}(E,b) = \dfrac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_{1,1}^{(s)}(E)}{14} - \dfrac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_{1,2}^{(s)}(E)}{14} - \dfrac{\sqrt{14}\mathbb{Q}_2^{(a)}(A_1)\mathbb{Q}_{1,1}^{(s)}(E)}{14}$

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

$\boxed{\text{z19}}$ $\quad \mathbb{Q}_{2,1}^{(c)}(E,1) = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E,1)\mathbb{Q}_0^{(s)}(A_1)}{2}$

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

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

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

$\boxed{\text{z23}}$ $\quad \mathbb{Q}_{3,1}^{(c)}(E,1) = \dfrac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_{1,1}^{(s)}(E)}{14} - \dfrac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_{1,2}^{(s)}(E)}{14} + \dfrac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_1)\mathbb{Q}_{1,1}^{(s)}(E)}{7}$

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

$\boxed{\text{z25}}$ $\quad \mathbb{Q}_{3,1}^{(c)}(E,2) = \dfrac{\mathbb{Q}_{2,1}^{(a)}(E,1)\mathbb{Q}_{1,1}^{(s)}(E)}{2} - \dfrac{\mathbb{Q}_{2,2}^{(a)}(E,1)\mathbb{Q}_{1,2}^{(s)}(E)}{2}$

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

z27 $\mathbb{G}_{2}^{(c)}(A_1) = -\dfrac{\sqrt{2}\,\mathbb{Q}_{2,1}^{(a)}(E,1)\mathbb{Q}_{1,1}^{(s)}(E)}{2} - \dfrac{\sqrt{2}\,\mathbb{Q}_{2,2}^{(a)}(E,1)\mathbb{Q}_{1,2}^{(s)}(E)}{2}$

- '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`

z5 $\mathbb{Q}_{0}^{(c)}(A_1) = \mathbb{Q}_{0}^{(a)}(A_1)\mathbb{Q}_{0}^{(b)}(A_1)$

z6 $\mathbb{Q}_{2}^{(c)}(A_1) = \mathbb{Q}_{2}^{(a)}(A_1)\mathbb{Q}_{0}^{(b)}(A_1)$

z7 $\mathbb{Q}_{3}^{(c)}(A_1) = \dfrac{\sqrt{2}\,\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_{1,1}^{(b)}(E)}{2} + \dfrac{\sqrt{2}\,\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$

z8 $\mathbb{Q}_{1}^{(c)}(A_2,a) = \dfrac{\sqrt{2}\,\mathbb{Q}_{2,1}^{(a)}(E,1)\mathbb{Q}_{1,2}^{(b)}(E)}{2} - \dfrac{\sqrt{2}\,\mathbb{Q}_{2,2}^{(a)}(E,1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$

z9 $\mathbb{Q}_{1}^{(c)}(A_2,b) = \dfrac{\sqrt{2}\,\mathbb{M}_{1,1}^{(a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2} - \dfrac{\sqrt{2}\,\mathbb{M}_{1,2}^{(a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2}$

z10 $\mathbb{Q}_{3}^{(c)}(A_2,2) = \dfrac{\sqrt{2}\,\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_{1,2}^{(b)}(E)}{2} - \dfrac{\sqrt{2}\,\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$

z13 $\mathbb{Q}_{1,1}^{(c)}(E,a) = \dfrac{\sqrt{2}\,\mathbb{Q}_{0}^{(a)}(A_1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$

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

z15 $\mathbb{Q}_{1,1}^{(c)}(E,b) = \dfrac{\sqrt{42}\,\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_{1,1}^{(b)}(E)}{14} - \dfrac{\sqrt{42}\,\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_{1,2}^{(b)}(E)}{14} - \dfrac{\sqrt{14}\,\mathbb{Q}_{2}^{(a)}(A_1)\mathbb{Q}_{1,1}^{(b)}(E)}{14}$

z28 $\mathbb{Q}_{1,2}^{(c)}(E,b) = -\dfrac{\sqrt{42}\,\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_{1,2}^{(b)}(E)}{14} - \dfrac{\sqrt{42}\,\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_{1,1}^{(b)}(E)}{14} - \dfrac{\sqrt{14}\,\mathbb{Q}_{2}^{(a)}(A_1)\mathbb{Q}_{1,2}^{(b)}(E)}{14}$

$$\boxed{\text{z29}} \quad \mathbb{Q}_{1,1}^{(c)}(E,c) = \frac{\mathbb{M}_{1,2}^{(a)}(E)\mathbb{T}_1^{(b)}(A_2)}{2} - \frac{\mathbb{M}_1^{(a)}(A_2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z30}} \quad \mathbb{Q}_{1,2}^{(c)}(E,c) = -\frac{\mathbb{M}_{1,1}^{(a)}(E)\mathbb{T}_1^{(b)}(A_2)}{2} + \frac{\mathbb{M}_1^{(a)}(A_2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

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

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

$$\boxed{\text{z33}} \quad \mathbb{Q}_{2,1}^{(c)}(E,2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z34}} \quad \mathbb{Q}_{2,2}^{(c)}(E,2) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z35}} \quad \mathbb{Q}_{3,1}^{(c)}(E,1) = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_{1,1}^{(b)}(E)}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_{1,2}^{(b)}(E)}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_1)\mathbb{Q}_{1,1}^{(b)}(E)}{7}$$

$$\boxed{\text{z36}} \quad \mathbb{Q}_{3,2}^{(c)}(E,1) = -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_{1,2}^{(b)}(E)}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_{1,1}^{(b)}(E)}{14} + \frac{\sqrt{21}\mathbb{Q}_2^{(a)}(A_1)\mathbb{Q}_{1,2}^{(b)}(E)}{7}$$

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

$$\boxed{\text{z38}} \quad \mathbb{Q}_{3,2}^{(c)}(E,2) = -\frac{\mathbb{Q}_{2,1}^{(a)}(E,1)\mathbb{Q}_{1,2}^{(b)}(E)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E,1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$$\boxed{\text{z39}} \quad \mathbb{G}_0^{(c)}(A_1) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{3} + \frac{\sqrt{3}\mathbb{M}_1^{(a)}(A_2)\mathbb{T}_1^{(b)}(A_2)}{3}$$

$$\boxed{\text{z40}} \quad \mathbb{G}_2^{(c)}(A_1,a) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E,1)\mathbb{Q}_{1,1}^{(b)}(E)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E,1)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$$\boxed{\text{z41}} \quad \mathbb{G}_2^{(c)}(A_1,b) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{6} + \frac{\sqrt{6}\mathbb{M}_1^{(a)}(A_2)\mathbb{T}_1^{(b)}(A_2)}{3}$$

$$\boxed{\text{z42}} \quad \mathbb{G}_{2,1}^{(c)}(E,1) = \frac{\mathbb{M}_{1,2}^{(a)}(E)\mathbb{T}_1^{(b)}(A_2)}{2} + \frac{\mathbb{M}_1^{(a)}(A_2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

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

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

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

— **Atomic SAMB** —————————————————————————————

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

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

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

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

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

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

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

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

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

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

━━━ **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`

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

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

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

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

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

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

--- **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 (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, $|v|$= 2.89426 (cartesian)

SL	vector (v)	center (c)	mapping	head	tail	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]