

# SAMB for “Te”

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- Group: No. 152  $D_3^4$   $P3_121$  [ trigonal ]
  - Associated point group: No. 18  $D_3 - 1$   $321$  (321 setting) [ trigonal ]
  - Generation condition
    - model type: **tight\_binding**
    - time-reversal type: **electric**
    - irrep: [A1]
    - spinless
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- Unit cell:
  - $a = 4.458$ ,  $b = 4.458$ ,  $c = 5.925$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 120.0$
- Lattice vectors:
  - $\mathbf{a}_1 = (4.458 \ 0 \ 0)$
  - $\mathbf{a}_2 = (-2.229 \ 3.86074125007103 \ 0)$
  - $\mathbf{a}_3 = (0 \ 0 \ 5.925)$

Table 1: High-symmetry line: A- $\Gamma$ -H-A-L-H-K- $\Gamma$ -M-K.

	symbol	position	symbol	position	symbol	position
	$\Gamma$	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	A	$\begin{pmatrix} 0 & 0 & \frac{1}{2} \end{pmatrix}$	M	$\begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$
	K	$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & 0 \end{pmatrix}$	H	$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{2} \end{pmatrix}$	L	$\begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$

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- Kets: dimension = 9

Table 2: Hilbert space for full matrix.

No.	ket	No.	ket	No.	ket	No.	ket	No.	ket
1	$p_x@A_1$	2	$p_y@A_1$	3	$p_z@A_1$	4	$p_x@A_2$	5	$p_y@A_2$
6	$p_z@A_2$	7	$p_x@A_3$	8	$p_y@A_3$	9	$p_z@A_3$		

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
S <sub>1</sub> [3a: .2.]	A <sub>1</sub>	$\begin{pmatrix} 0.274 & 0 & \frac{1}{3} \end{pmatrix}$	[1,2]
	A <sub>2</sub>	$\begin{pmatrix} 0.726 & 0.726 & 0 \end{pmatrix}$	[3,6]
	A <sub>3</sub>	$\begin{pmatrix} 0 & 0.274 & \frac{2}{3} \end{pmatrix}$	[4,5]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	$n$	#	$\mathbf{b@c}$	mapping
B <sub>1</sub> [3b: .2.]	b <sub>1</sub>	A <sub>2</sub>	A <sub>1</sub>	1	1	$\begin{pmatrix} -0.548 & -0.274 & -\frac{1}{3} \end{pmatrix} @ \begin{pmatrix} 0 & 0.863 & \frac{1}{6} \end{pmatrix}$	[1,-3]
	b <sub>2</sub>	A <sub>3</sub>	A <sub>1</sub>	1	1	$\begin{pmatrix} -0.274 & 0.274 & \frac{1}{3} \end{pmatrix} @ \begin{pmatrix} 0.137 & 0.137 & \frac{1}{2} \end{pmatrix}$	[2,-5]
	b <sub>3</sub>	A <sub>3</sub>	A <sub>2</sub>	1	1	$\begin{pmatrix} 0.274 & 0.548 & -\frac{1}{3} \end{pmatrix} @ \begin{pmatrix} 0.863 & 0 & \frac{5}{6} \end{pmatrix}$	[-4,6]

- SAMB:

$$\boxed{\text{No. 1}} \quad \hat{Q}_0^{(A_1)} [M_1, S_1]$$

$$\hat{Z}_1 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A_1)}]$$

$$\boxed{\text{No. 2}} \quad \hat{\mathbb{Q}}_2^{(A_1)} [\mathbb{M}_1, \mathbb{S}_1]$$

$$\hat{\mathbb{Z}}_2 = \mathbb{X}_2[\mathbb{Q}_2^{(a,A_1)}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A_1)}]$$

$$\boxed{\text{No. 3}} \quad \hat{\mathbb{G}}_2^{(A_1)} [\mathbb{M}_1, \mathbb{S}_1]$$

$$\hat{\mathbb{Z}}_3 = -\frac{\sqrt{2}\mathbb{X}_3[\mathbb{Q}_{2,0}^{(a,E,1)}] \otimes \mathbb{Y}_2[\mathbb{Q}_{1,0}^{(s,E)}]}{2} - \frac{\sqrt{2}\mathbb{X}_4[\mathbb{Q}_{2,1}^{(a,E,1)}] \otimes \mathbb{Y}_3[\mathbb{Q}_{1,1}^{(s,E)}]}{2}$$

$$\boxed{\text{No. 4}} \quad \hat{\mathbb{Q}}_3^{(A_1)} [\mathbb{M}_1, \mathbb{S}_1]$$

$$\hat{\mathbb{Z}}_4 = \frac{\sqrt{2}\mathbb{X}_5[\mathbb{Q}_{2,0}^{(a,E,2)}] \otimes \mathbb{Y}_2[\mathbb{Q}_{1,0}^{(s,E)}]}{2} + \frac{\sqrt{2}\mathbb{X}_6[\mathbb{Q}_{2,1}^{(a,E,2)}] \otimes \mathbb{Y}_3[\mathbb{Q}_{1,1}^{(s,E)}]}{2}$$

$$\boxed{\text{No. 5}} \quad \hat{\mathbb{Q}}_0^{(A_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbb{Z}}_5 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_1)}]$$

$$\boxed{\text{No. 6}} \quad \hat{\mathbb{Q}}_2^{(A_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbb{Z}}_6 = \mathbb{X}_2[\mathbb{Q}_2^{(a,A_1)}] \otimes \mathbb{Y}_4[\mathbb{Q}_0^{(b,A_1)}]$$

$$\boxed{\text{No. 7}} \quad \hat{\mathbb{G}}_2^{(A_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbb{Z}}_7 = -\frac{\sqrt{2}\mathbb{X}_3[\mathbb{Q}_{2,0}^{(a,E,1)}] \otimes \mathbb{Y}_5[\mathbb{Q}_{1,0}^{(b,E)}]}{2} - \frac{\sqrt{2}\mathbb{X}_4[\mathbb{Q}_{2,1}^{(a,E,1)}] \otimes \mathbb{Y}_6[\mathbb{Q}_{1,1}^{(b,E)}]}{2}$$

$$\boxed{\text{No. 8}} \quad \hat{\mathbb{Q}}_3^{(A_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbb{Z}}_8 = \frac{\sqrt{2}\mathbb{X}_5[\mathbb{Q}_{2,0}^{(a,E,2)}] \otimes \mathbb{Y}_5[\mathbb{Q}_{1,0}^{(b,E)}]}{2} + \frac{\sqrt{2}\mathbb{X}_6[\mathbb{Q}_{2,1}^{(a,E,2)}] \otimes \mathbb{Y}_6[\mathbb{Q}_{1,1}^{(b,E)}]}{2}$$

$$\boxed{\text{No. 9}} \quad \hat{\mathbb{G}}_0^{(A_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbb{Z}}_9 = \frac{\sqrt{3}\mathbb{X}_7[\mathbb{M}_1^{(a,A_2)}] \otimes \mathbb{Y}_7[\mathbb{T}_1^{(b,A_2)}]}{3} - \frac{\sqrt{3}\mathbb{X}_8[\mathbb{M}_{1,0}^{(a,E)}] \otimes \mathbb{Y}_9[\mathbb{T}_{1,1}^{(b,E)}]}{3} + \frac{\sqrt{3}\mathbb{X}_9[\mathbb{M}_{1,1}^{(a,E)}] \otimes \mathbb{Y}_8[\mathbb{T}_{1,0}^{(b,E)}]}{3}$$

$$\boxed{\text{No. 10}} \quad \hat{\mathbb{G}}_2^{(A_1)} [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbb{Z}}_{10} = \frac{\sqrt{6}\mathbb{X}_7[\mathbb{M}_1^{(a,A_2)}] \otimes \mathbb{Y}_7[\mathbb{T}_1^{(b,A_2)}]}{3} + \frac{\sqrt{6}\mathbb{X}_8[\mathbb{M}_{1,0}^{(a,E)}] \otimes \mathbb{Y}_9[\mathbb{T}_{1,1}^{(b,E)}]}{6} - \frac{\sqrt{6}\mathbb{X}_9[\mathbb{M}_{1,1}^{(a,E)}] \otimes \mathbb{Y}_8[\mathbb{T}_{1,0}^{(b,E)}]}{6}$$

Table 5: Atomic SAMB group.

group	bra	ket
$M_1$	$p_x, p_y, p_z$	$p_x, p_y, p_z$

Table 6: Atomic SAMB.

symbol	type	group	form
$X_1$	$Q_0^{(a,A_1)}$	$M_1$	$\begin{pmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$
$X_2$	$Q_2^{(a,A_1)}$	$M_1$	$\begin{pmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{pmatrix}$
$X_3$	$Q_{2,0}^{(a,E,1)}$	$M_1$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
$X_4$	$Q_{2,1}^{(a,E,1)}$	$M_1$	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{2}}{2} \\ 0 & 0 & 0 \\ -\frac{\sqrt{2}}{2} & 0 & 0 \end{pmatrix}$
$X_5$	$Q_{2,0}^{(a,E,2)}$	$M_1$	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$X_6$	$Q_{2,1}^{(a,E,2)}$	$M_1$	$\begin{pmatrix} 0 & -\frac{\sqrt{2}}{2} & 0 \\ -\frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$X_7$	$M_1^{(a,A_2)}$	$M_1$	$\begin{pmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

*continued ...*

Table 6

symbol	type	group	form
$\mathbb{X}_8$	$\mathbb{M}_{1,0}^{(a,E)}$	$M_1$	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_9$	$\mathbb{M}_{1,1}^{(a,E)}$	$M_1$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & \frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
$\mathbb{Y}_1$	$\mathbb{Q}_0^{(s,A_1)}$	$S_1$	$\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \end{pmatrix}$
$\mathbb{Y}_2$	$\mathbb{Q}_{1,0}^{(s,E)}$	$S_1$	$\begin{pmatrix} \frac{\sqrt{6}}{3} & -\frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{6} \end{pmatrix}$
$\mathbb{Y}_3$	$\mathbb{Q}_{1,1}^{(s,E)}$	$S_1$	$\begin{pmatrix} 0 & -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{Y}_4$	$\mathbb{Q}_0^{(b,A_1)}$	$B_1$	$\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \end{pmatrix}$
$\mathbb{Y}_5$	$\mathbb{Q}_{1,0}^{(b,E)}$	$B_1$	$\begin{pmatrix} \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & -\frac{\sqrt{6}}{3} \end{pmatrix}$
$\mathbb{Y}_6$	$\mathbb{Q}_{1,1}^{(b,E)}$	$B_1$	$\begin{pmatrix} -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
$\mathbb{Y}_7$	$\mathbb{T}_1^{(b,A_2)}$	$B_1$	$\begin{pmatrix} \frac{\sqrt{3}i}{3} & -\frac{\sqrt{3}i}{3} & \frac{\sqrt{3}i}{3} \end{pmatrix}$
$\mathbb{Y}_8$	$\mathbb{T}_{1,0}^{(b,E)}$	$B_1$	$\begin{pmatrix} \frac{\sqrt{2}i}{2} & \frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$
$\mathbb{Y}_9$	$\mathbb{T}_{1,1}^{(b,E)}$	$B_1$	$\begin{pmatrix} \frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{6} & -\frac{\sqrt{6}i}{3} \end{pmatrix}$

Table 8: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_1)}$	0	$A_1$	—	—	1
2	$\mathbb{Q}_1^{(A_2)}$	1	$A_2$	—	—	$z$
3	$\mathbb{Q}_{1,0}^{(E)}$	1	$E$	—	0	$x$
4	$\mathbb{Q}_{1,1}^{(E)}$	1	$E$	—	1	$y$
5	$\mathbb{Q}_2^{(A_1)}$	2	$A_1$	—	—	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
6	$\mathbb{Q}_{2,0}^{(E,1)}$	2	$E$	1	0	$\sqrt{3}yz$
7	$\mathbb{Q}_{2,1}^{(E,1)}$	2	$E$	1	1	$-\sqrt{3}xz$
8	$\mathbb{Q}_{2,0}^{(E,2)}$	2	$E$	2	0	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
9	$\mathbb{Q}_{2,1}^{(E,2)}$	2	$E$	2	1	$-\sqrt{3}xy$

Table 9: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_1^{(A_2)}$	1	$A_2$	—	—	$Z$
2	$\mathbb{G}_{1,0}^{(E)}$	1	$E$	—	0	$-Y$
3	$\mathbb{G}_{1,1}^{(E)}$	1	$E$	—	1	$X$

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- Group info.: Generator =  $\{3_{001}^+|00\frac{1}{3}\}$ ,  $\{2_{110}|0\}$

Table 10: Conjugacy class (point-group part).

rep. SO	symmetry operations
$\{1 0\}$	$\{1 0\}$
$\{2_{100} 00\frac{2}{3}\}$	$\{2_{100} 00\frac{2}{3}\}$ , $\{2_{010} 00\frac{1}{3}\}$ , $\{2_{110} 0\}$

*continued ...*

Table 10

rep. SO	symmetry operations
$\{3_{001}^+ 00\frac{1}{3}\}$	$\{3_{001}^+ 00\frac{1}{3}\}, \{3_{001}^- 00\frac{2}{3}\}$

Table 11: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	$\{1 0\}$	2	$\{2_{100} 00\frac{2}{3}\}$	3	$\{2_{010} 00\frac{1}{3}\}$	4	$\{2_{110} 0\}$	5	$\{3_{001}^+ 00\frac{1}{3}\}$
6	$\{3_{001}^- 00\frac{2}{3}\}$								

Table 12: Character table (point-group part).

	1	$2_{100}$	$3_{001}^+$
$A_1$	1	1	1
$A_2$	1	-1	1
$E$	2	0	-1

Table 13: Parity conversion.

$\leftrightarrow$	$\leftrightarrow$	$\leftrightarrow$
$A_1 (A_1)$	$A_2 (A_2)$	$E (E)$

Table 14: Symmetric product,  $[\Gamma \otimes \Gamma']_+$ .

	$A_1$	$A_2$	$E$
$A_1$	$A_1$	$A_2$	$E$
$A_2$		$A_1$	$E$
$E$			$A_1 + E$

Table 15: Anti-symmetric product,  $[\Gamma \otimes \Gamma']_-$ .

$A_1$	$A_2$	$E$
$-$	$-$	$A_2$

Table 16: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix} 1 & -1 & 1 \end{pmatrix}$	2	$\begin{pmatrix} 2 & 1 & -1 \end{pmatrix}$	3	$\begin{pmatrix} -1 & -2 & -1 \end{pmatrix}$	4	$\begin{pmatrix} -1 & 1 & -1 \end{pmatrix}$
5	$\begin{pmatrix} 1 & 2 & 1 \end{pmatrix}$	6	$\begin{pmatrix} -2 & -1 & 1 \end{pmatrix}$				

Table 17: Virtual-cluster basis.

symbol	1	2	3	4	5	6
$\mathbb{Q}_0^{(A_1)}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$
$\mathbb{Q}_1^{(A_2)}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{6}$
$\mathbb{Q}_{1,0}^{(E)}$	$\frac{1}{2}$	$\frac{1}{2}$	0	$-\frac{1}{2}$	0	$-\frac{1}{2}$
$\mathbb{Q}_{1,1}^{(E)}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{3}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$	$-\frac{\sqrt{3}}{6}$

*continued ...*



Table 17

symbol	1	2	3	4	5	6
$Q_{2,0}^{(E,1)}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$	$-\frac{\sqrt{3}}{6}$
$Q_{2,1}^{(E,1)}$	$-\frac{1}{2}$	$\frac{1}{2}$	0	$-\frac{1}{2}$	0	$\frac{1}{2}$