SAMB for “Te”

Generated on 2023-09-27 01:33 by MultiPie 1.1.14

- 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`

- Unit cell:
  $a=4.458,\ b=4.458,\ c=5.925,\ \alpha=90.0,\ \beta=90.0,\ \gamma=120.0$
- Lattice vectors:
  $\boldsymbol{a}_1=\begin{pmatrix}4.458 & 0 & 0\end{pmatrix}$
  $\boldsymbol{a}_2=\begin{pmatrix}-2.229 & 3.86074125007103 & 0\end{pmatrix}$
  $\boldsymbol{a}_3=\begin{pmatrix}0 & 0 & 5.925\end{pmatrix}$

Table 1: High-symmetry line: A-Γ-H-A-L-H-K-Γ-M-K.

symbol	position	symbol	position	symbol	position
Γ	$\begin{pmatrix}0 & 0 & 0\end{pmatrix}$	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	$\begin{pmatrix}\frac{1}{2} & 0 & \frac{1}{2}\end{pmatrix}$

- 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_1 [3a: .2.]	A_1	$\begin{pmatrix} 0.274 & 0 & \frac{1}{3} \end{pmatrix}$	[1,2]
	A_2	$\begin{pmatrix} 0.726 & 0.726 & 0 \end{pmatrix}$	[3,6]
	A_3	$\begin{pmatrix} 0 & 0.274 & \frac{2}{3} \end{pmatrix}$	[4,5]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	$\boldsymbol{b}$@$\boldsymbol{c}$	mapping
B_1 [3b: .2.]	b_1	A_2	A_1	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_2	A_3	A_1	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_3	A_3	A_2	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:

$\boxed{\text{No. 1}}$ $\hat{\mathbb{Q}}_0^{(A_1)}$ $[\mathrm{M}_1, \mathrm{S}_1]$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
$\mathbb{X}_1$	$\mathbb{Q}_0^{(a,A_1)}$	M_1	$\begin{pmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$
$\mathbb{X}_2$	$\mathbb{Q}_2^{(a,A_1)}$	M_1	$\begin{pmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{pmatrix}$
$\mathbb{X}_3$	$\mathbb{Q}_{2,0}^{(a,E,1)}$	M_1	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
$\mathbb{X}_4$	$\mathbb{Q}_{2,1}^{(a,E,1)}$	M_1	$\begin{pmatrix} 0 & 0 & -\frac{\sqrt{2}}{2} \\ 0 & 0 & 0 \\ -\frac{\sqrt{2}}{2} & 0 & 0 \end{pmatrix}$
$\mathbb{X}_5$	$\mathbb{Q}_{2,0}^{(a,E,2)}$	M_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_6$	$\mathbb{Q}_{2,1}^{(a,E,2)}$	M_1	$\begin{pmatrix} 0 & -\frac{\sqrt{2}}{2} & 0 \\ -\frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
$\mathbb{X}_7$	$\mathbb{M}_1^{(a,A_2)}$	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

- 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
$\mathbb{Q}_{2,0}^{(E,1)}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$	$-\frac{\sqrt{3}}{6}$
$\mathbb{Q}_{2,1}^{(E,1)}$	$-\frac{1}{2}$	$\frac{1}{2}$	0	$-\frac{1}{2}$	0	$\frac{1}{2}$