

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: **phonon**
 - 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:
 $\mathbf{a}_1 = (4.458 \ 0 \ 0)$
 $\mathbf{a}_2 = (-2.229 \ 3.86074125007103 \ 0)$
 $\mathbf{a}_3 = (0 \ 0 \ 5.925)$

Table 1: High-symmetry line: A- 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 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	#	$\mathbf{b@c}$	mapping
B ₁ 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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned} \hat{\mathbb{Z}}_5(\mathbf{k}) = & \frac{\sqrt{6}\mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_4[\mathbb{Q}_0^{(u,A_1)}] \otimes \mathbb{F}_1[\mathbb{Q}_0^{(k,A_1)}]}{6} + \frac{\sqrt{6}\mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_5[\mathbb{Q}_{1,0}^{(u,E)}] \otimes \mathbb{F}_2[\mathbb{Q}_{1,0}^{(k,E)}]}{6} + \frac{\sqrt{6}\mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_6[\mathbb{Q}_{1,1}^{(u,E)}] \otimes \mathbb{F}_3[\mathbb{Q}_{1,1}^{(k,E)}]}{6} \\ & - \frac{\sqrt{6}\mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_7[\mathbb{T}_1^{(u,A_2)}] \otimes \mathbb{F}_4[\mathbb{T}_1^{(k,A_2)}]}{6} - \frac{\sqrt{6}\mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_8[\mathbb{T}_{1,0}^{(u,E)}] \otimes \mathbb{F}_5[\mathbb{T}_{1,0}^{(k,E)}]}{6} - \frac{\sqrt{6}\mathbb{X}_1[\mathbb{Q}_0^{(a,A_1)}] \otimes \mathbb{U}_9[\mathbb{T}_{1,1}^{(u,E)}] \otimes \mathbb{F}_6[\mathbb{T}_{1,1}^{(k,E)}]}{6} \end{aligned}$$

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

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

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	$\begin{pmatrix} 0 & -\frac{\sqrt{2}}{2} & 0 \\ -\frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

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	$\begin{pmatrix} -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 \end{pmatrix}$

Table 8: Uniform SAMB.

symbol	type	cluster	form
\mathbb{U}_1	$\mathbb{Q}_0^{(s,A_1)}$	S_1	$\begin{pmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{pmatrix}$
\mathbb{U}_2	$\mathbb{Q}_{1,0}^{(s,E)}$	S_1	$\begin{pmatrix} \frac{\sqrt{6}}{3} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{U}_3	$\mathbb{Q}_{1,1}^{(s,E)}$	S_1	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{U}_4	$\mathbb{Q}_0^{(u,A_1)}$	B_1	$\begin{pmatrix} 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \\ \frac{\sqrt{6}}{6} & 0 & \frac{\sqrt{6}}{6} \\ \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} & 0 \end{pmatrix}$
\mathbb{U}_5	$\mathbb{Q}_{1,0}^{(u,E)}$	B_1	$\begin{pmatrix} 0 & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}}{6} \\ \frac{\sqrt{3}}{6} & 0 & -\frac{\sqrt{3}}{3} \\ \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}}{3} & 0 \end{pmatrix}$

continued ...

Table 8

symbol	type	cluster	form
\mathbb{U}_6	$\mathbb{Q}_{1,1}^{(u,E)}$	B_1	$\begin{pmatrix} 0 & -\frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 \end{pmatrix}$
\mathbb{U}_7	$\mathbb{T}_1^{(u,A_2)}$	B_1	$\begin{pmatrix} 0 & -\frac{\sqrt{6}i}{6} & \frac{\sqrt{6}i}{6} \\ \frac{\sqrt{6}i}{6} & 0 & -\frac{\sqrt{6}i}{6} \\ -\frac{\sqrt{6}i}{6} & \frac{\sqrt{6}i}{6} & 0 \end{pmatrix}$
\mathbb{U}_8	$\mathbb{T}_{1,0}^{(u,E)}$	B_1	$\begin{pmatrix} 0 & -\frac{i}{2} & -\frac{i}{2} \\ \frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 \end{pmatrix}$
\mathbb{U}_9	$\mathbb{T}_{1,1}^{(u,E)}$	B_1	$\begin{pmatrix} 0 & -\frac{\sqrt{3}i}{6} & \frac{\sqrt{3}i}{6} \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}i}{3} \\ -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}i}{3} & 0 \end{pmatrix}$

Table 9: Structure SAMB.

symbol	type	cluster	form
\mathbb{F}_1	$\mathbb{Q}_0^{(k,A_1)}$	B_1	$\frac{\sqrt{6}c_{001}}{3} + \frac{\sqrt{6}c_{002}}{3} + \frac{\sqrt{6}c_{003}}{3}$
\mathbb{F}_2	$\mathbb{Q}_{1,0}^{(k,E)}$	B_1	$\frac{\sqrt{3}c_{001}}{3} + \frac{\sqrt{3}c_{002}}{3} - \frac{2\sqrt{3}c_{003}}{3}$
\mathbb{F}_3	$\mathbb{Q}_{1,1}^{(k,E)}$	B_1	$-c_{001} + c_{002}$
\mathbb{F}_4	$\mathbb{T}_1^{(k,A_2)}$	B_1	$\frac{\sqrt{6}s_{001}}{3} - \frac{\sqrt{6}s_{002}}{3} + \frac{\sqrt{6}s_{003}}{3}$
\mathbb{F}_5	$\mathbb{T}_{1,0}^{(k,E)}$	B_1	$s_{001} + s_{002}$
\mathbb{F}_6	$\mathbb{T}_{1,1}^{(k,E)}$	B_1	$\frac{\sqrt{3}s_{001}}{3} - \frac{\sqrt{3}s_{002}}{3} - \frac{2\sqrt{3}s_{003}}{3}$

Table 10: 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	$-\sqrt{3}xy$

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

Table 11: Conjugacy class (point-group part).

rep. SO	symmetry operations
$\{1 0\}$	$\{1 0\}$
$\{2_{100} 00\frac{2}{3}\}$	$\{2_{100} 00\frac{2}{3}\}, \{2_{010} 00\frac{1}{3}\}, \{2_{110} 0\}$
$\{3_{001}^+ 00\frac{1}{3}\}$	$\{3_{001}^+ 00\frac{1}{3}\}, \{3_{001}^- 00\frac{2}{3}\}$

Table 12: 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 13: 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 14: Parity conversion.

\leftrightarrow	\leftrightarrow	\leftrightarrow
A ₁ (A ₁)	A ₂ (A ₂)	E (E)

Table 15: 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 16: Anti-symmetric product, $[\Gamma \otimes \Gamma']_-$.

A ₁	A ₂	E
-	-	A ₂

Table 17: 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 18: 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	$-\frac{1}{2}$
$\mathbb{Q}_{1,1}^{(E)}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{3}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$	$-\frac{\sqrt{3}}{6}$
$\mathbb{Q}_{2,0}^{(E,1)}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{3}$	$-\frac{\sqrt{3}}{6}$
$\mathbb{Q}_{2,1}^{(E,1)}$	$-\frac{1}{2}$	$\frac{1}{2}$	0	$-\frac{1}{2}$	0	$\frac{1}{2}$