

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 [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	#	$\mathbf{b@c}$	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:

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

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

$$\boxed{\text{No. 2}} \quad \hat{Q}_2^{(A_1)} [M_1, S_1]$$

$$\hat{Z}_2 = X_2[Q_2^{(a, A_1)}] \otimes Y_1[Q_0^{(s, A_1)}]$$

$$\boxed{\text{No. 3}} \quad \hat{G}_2^{(A_1)} [M_1, S_1]$$

$$\hat{Z}_3 = -\frac{\sqrt{2}X_3[Q_{2,0}^{(a, E, 1)}] \otimes Y_2[Q_{1,0}^{(s, E)}]}{2} - \frac{\sqrt{2}X_4[Q_{2,1}^{(a, E, 1)}] \otimes Y_3[Q_{1,1}^{(s, E)}]}{2}$$

$$\boxed{\text{No. 4}} \quad \hat{Q}_3^{(A_1)} [M_1, S_1]$$

$$\hat{Z}_4 = \frac{\sqrt{2}X_5[Q_{2,0}^{(a, E, 2)}] \otimes Y_2[Q_{1,0}^{(s, E)}]}{2} + \frac{\sqrt{2}X_6[Q_{2,1}^{(a, E, 2)}] \otimes Y_3[Q_{1,1}^{(s, E)}]}{2}$$

$$\boxed{\text{No. 5}} \quad \hat{Q}_0^{(A_1)} [M_1, B_1]$$

$$\hat{Z}_5 = X_1[Q_0^{(a, A_1)}] \otimes Y_4[Q_0^{(b, A_1)}]$$

$$\boxed{\text{No. 6}} \quad \hat{Q}_2^{(A_1)} [M_1, B_1]$$

$$\hat{Z}_6 = X_2[Q_2^{(a, A_1)}] \otimes Y_4[Q_0^{(b, A_1)}]$$

$$\boxed{\text{No. 7}} \quad \hat{G}_2^{(A_1)} [M_1, B_1]$$

$$\hat{Z}_7 = -\frac{\sqrt{2}X_3[Q_{2,0}^{(a, E, 1)}] \otimes Y_5[Q_{1,0}^{(b, E)}]}{2} - \frac{\sqrt{2}X_4[Q_{2,1}^{(a, E, 1)}] \otimes Y_6[Q_{1,1}^{(b, E)}]}{2}$$

$$\boxed{\text{No. 8}} \quad \hat{Q}_3^{(A_1)} [M_1, B_1]$$

$$\hat{Z}_8 = \frac{\sqrt{2}X_5[Q_{2,0}^{(a, E, 2)}] \otimes Y_5[Q_{1,0}^{(b, E)}]}{2} + \frac{\sqrt{2}X_6[Q_{2,1}^{(a, E, 2)}] \otimes Y_6[Q_{1,1}^{(b, E)}]}{2}$$

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: Polar harmonics.

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

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

Table 9: 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 10: 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 11: 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 12: Parity conversion.

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

Table 13: 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 14: Anti-symmetric product, $[\Gamma \otimes \Gamma']_-$.

A_1	A_2	E
$-$	$-$	A_2

Table 15: 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 16: 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 16

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	$\frac{1}{2}$