

# Model for “kappaET”

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## General Condition

- Basis type: **lgs**
- SAMB selection:
  - Type: **[Q, G]**
  - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
  - Irrep.: **[A<sub>1</sub>, A<sub>2</sub>, B<sub>1</sub>, B<sub>2</sub>]**
  - Spin (s): **[0, 1]**
- Atomic selection:
  - Type: **[Q, G, M, T]**
  - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
  - Irrep.: **[A<sub>1</sub>, A<sub>2</sub>, B<sub>1</sub>, B<sub>2</sub>]**
  - Spin (s): **[0, 1]**
- Site-cluster selection:
  - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
  - Irrep.: **[A<sub>1</sub>, A<sub>2</sub>, B<sub>1</sub>, B<sub>2</sub>]**
- Bond-cluster selection:
  - Type: **[Q, G, M, T]**
  - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
  - Irrep.: **[A<sub>1</sub>, A<sub>2</sub>, B<sub>1</sub>, B<sub>2</sub>]**
- Max. neighbor: **10**
- Search cell range: **(-2, 3), (-2, 3), (-2, 3)**
- Toroidal priority: **false**

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## Group and Unit Cell

- Group: SG No. 32  $C_{2v}^8$  *Pba2* [ orthorhombic ]
- Associated point group: PG No. 32  $C_{2v}$  *mm2* [ orthorhombic ]
- Unit cell:
  - $a = 1.00000$ ,  $b = 1.20000$ ,  $c = 1.00000$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 90.0$
- Lattice vectors (conventional cell):
  - $\mathbf{a}_1 = [ 1.00000, 0.00000, 0.00000 ]$
  - $\mathbf{a}_2 = [ 0.00000, 1.20000, 0.00000 ]$
  - $\mathbf{a}_3 = [ 0.00000, 0.00000, 1.00000 ]$

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## Symmetry Operation

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Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	$\{1 0\}$	2	$\{2_{001} 0\}$	3	$\{m_{010} \frac{1}{2}\frac{1}{2}0\}$	4	$\{m_{100} \frac{1}{2}\frac{1}{2}0\}$		

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## Harmonics

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Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$Q_0(A_1)$	$A_1$	0	$Q, T$	-	-	1
2	$Q_1(A_1)$	$A_1$	1	$Q, T$	-	-	$z$
3	$G_2(A_1)$	$A_1$	2	$G, M$	-	-	$\sqrt{3}xy$
4	$G_0(A_2)$	$A_2$	0	$G, M$	-	-	1
5	$G_1(A_2)$	$A_2$	1	$G, M$	-	-	$z$
6	$G_2(A_2, 2)$	$A_2$	2	$G, M$	2	-	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
7	$Q_2(A_2)$	$A_2$	2	$Q, T$	-	-	$\sqrt{3}xy$
8	$G_1(B_1)$	$B_1$	1	$G, M$	-	-	$y$
9	$Q_1(B_1)$	$B_1$	1	$Q, T$	-	-	$x$

*continued ...*

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
10	$\mathbb{Q}_2(B_1)$	$B_1$	2	$Q, T$	-	-	$\sqrt{3}xz$
11	$\mathbb{G}_1(B_2)$	$B_2$	1	$G, M$	-	-	$x$
12	$\mathbb{Q}_1(B_2)$	$B_2$	1	$Q, T$	-	-	$y$
13	$\mathbb{Q}_2(B_2)$	$B_2$	2	$Q, T$	-	-	$\sqrt{3}yz$

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Basis in full matrix

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Table 3: dimension = 8

#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)
0	$ s, \uparrow\rangle @A(1)$	1	$ s, \downarrow\rangle @A(1)$	2	$ s, \uparrow\rangle @A(2)$	3	$ s, \downarrow\rangle @A(2)$	4	$ s, \uparrow\rangle @A(3)$
5	$ s, \downarrow\rangle @A(3)$	6	$ s, \uparrow\rangle @A(4)$	7	$ s, \downarrow\rangle @A(4)$				

Table 4: Atomic basis (orbital part only)

orbital	definition
$ s\rangle$	1

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## SAMB

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28 (all 44) SAMBs

- 'A' site-cluster

- \* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$
- \* ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$
- \* wyckoff: **4c**

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

$$\boxed{\text{z13}} \quad \mathbb{Q}_2^{(c)}(A_2) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_2^{(s)}(A_2)$$

$$\boxed{\text{z25}} \quad \mathbb{Q}_1^{(c)}(B_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_1^{(s)}(B_1)$$

$$\boxed{\text{z35}} \quad \mathbb{Q}_1^{(c)}(B_2) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_1^{(s)}(B_2)$$

- 'A'-'A' bond-cluster

- \* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$
- \* ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$
- \* wyckoff: **2a02a**

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

$$\boxed{\text{z3}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_1) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_1)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_2)}{2}$$

$$\boxed{\text{z4}} \quad \mathbb{G}_2^{(1,-1;c)}(A_1) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_1)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_2)}{2}$$

$$\boxed{\text{z14}} \quad \mathbb{Q}_2^{(c)}(A_2) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_2^{(b)}(A_2)$$

$$\boxed{\text{z15}} \quad \mathbb{G}_0^{(1,-1;c)}(A_2) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_2)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_1)}{2}$$

$$\boxed{\text{z16}} \quad \mathbb{G}_2^{(1,-1;c)}(A_2, 2) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_2)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_1)}{2}$$

$$\boxed{\text{z26}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_1) = -\mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_1^{(b)}(B_2)$$

$$\boxed{\text{z36}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_2) = \mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_1^{(b)}(B_1)$$

• 'A'-'A' bond-cluster

\* bra:  $\langle s, \uparrow |, \langle s, \downarrow |$

\* ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$

\* wyckoff: **4a@4c**

$$\boxed{\text{z5}} \quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(b)}(A_1)$$

$$\boxed{\text{z6}} \quad \mathbb{Q}_0^{(1,-1;c)}(A_1) = \mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{M}_1^{(b)}(A_2)$$

$$\boxed{\text{z7}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_1) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_1)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_2)}{2}$$

$$\boxed{\text{z8}} \quad \mathbb{G}_2^{(1,-1;c)}(A_1) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_1)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_2)}{2}$$

$$\boxed{\text{z17}} \quad \mathbb{Q}_2^{(c)}(A_2) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_2^{(b)}(A_2)$$

$$\boxed{\text{z18}} \quad \mathbb{G}_0^{(1,-1;c)}(A_2) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_2)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_1)}{2}$$

$$\boxed{\text{z19}} \quad \mathbb{G}_1^{(1,-1;c)}(A_2) = \mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_0^{(b)}(A_1)$$

$$\boxed{\text{z20}} \quad \mathbb{G}_2^{(1,-1;c)}(A_2, 2) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_2)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_1)}{2}$$

$$\boxed{\text{z27}} \quad \mathbb{Q}_1^{(c)}(B_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_1^{(b)}(B_1)$$

$$\boxed{\text{z28}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_1) = -\mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_1^{(b)}(B_2)$$

$$\boxed{\text{z29}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_1) = \mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{M}_1^{(b)}(A_2)$$

$$\boxed{\text{z30}} \quad \mathbb{G}_1^{(1,-1;c)}(B_1) = \mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_0^{(b)}(A_1)$$

$$\boxed{\text{z37}} \quad \mathbb{Q}_1^{(c)}(B_2) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_1^{(b)}(B_2)$$

$$\boxed{\text{z38}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_2) = \mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_1^{(b)}(B_1)$$

$$\boxed{\text{z39}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_2) = \mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{M}_1^{(b)}(A_2)$$

$$\boxed{\text{z40}} \quad \mathbb{G}_1^{(1,-1;c)}(B_2) = \mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_0^{(b)}(A_1)$$

\* common SAMBs

(z5, z9), (z6, z10), (z7, z11), (z8, z12), (z17, z21), (z18, z22), (z19, z23), (z20, z24), (z27, z31), (z28, z32), (z29, z33), (z30, z34), (z37, z41), (z38, z42), (z39, z43), (z40, z44)

## — Atomic SAMB —

- bra:  $\langle s, \uparrow |, \langle s, \downarrow |$
- ket:  $|s, \uparrow\rangle, |s, \downarrow\rangle$

$$\boxed{\text{x1}} \quad \mathbb{Q}_0^{(a)}(A_1) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$$

$$\boxed{\text{x2}} \quad \mathbb{M}_1^{(1,-1;a)}(A_2) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{bmatrix}$$

$$\boxed{\text{x3}} \quad \mathbb{M}_1^{(1,-1;a)}(B_1) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$$

$$\boxed{\text{x4}} \quad \mathbb{M}_1^{(1,-1;a)}(B_2) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$$

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## Cluster SAMB

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- Site cluster

\*\* Wyckoff: 4c

$$\boxed{\text{y1}} \quad \mathbb{Q}_0^{(s)}(A_1) = \left[ \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right]$$

$$\boxed{\text{y2}} \quad \mathbb{Q}_2^{(s)}(A_2) = \left[ \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{\text{y3}} \quad \mathbb{Q}_1^{(s)}(B_1) = \left[ \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{\text{y4}} \quad \mathbb{Q}_1^{(s)}(B_2) = \left[ \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2} \right]$$

- Bond cluster

\*\* Wyckoff: 2a@2a

$$\boxed{\text{y5}} \quad \mathbb{Q}_0^{(s)}(A_1) = \left[ \frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2} \right]$$

$$\boxed{\text{y6}} \quad \mathbb{Q}_2^{(s)}(A_2) = \left[ \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

$$\boxed{\text{y7}} \quad \mathbb{T}_1^{(s)}(B_1) = \left[ \frac{\sqrt{2}i}{2}, \frac{\sqrt{2}i}{2} \right]$$

$$\boxed{\text{y8}} \quad \mathbb{T}_1^{(s)}(B_2) = \left[ \frac{\sqrt{2}i}{2}, -\frac{\sqrt{2}i}{2} \right]$$

\*\* Wyckoff: 4a@4c

$$\boxed{\text{y9}} \quad \mathbb{Q}_0^{(s)}(A_1) = \left[ \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right]$$

$$\boxed{\text{y10}} \quad \mathbb{T}_0^{(s)}(A_1) = \left[ \frac{i}{2}, \frac{i}{2}, \frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{\text{y11}} \quad \mathbb{M}_1^{(s)}(A_2) = \left[ \frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, -\frac{i}{2} \right]$$

$$\boxed{\text{y12}} \quad \mathbb{Q}_2^{(s)}(A_2) = \left[ \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{\text{y13}} \quad \mathbb{Q}_1^{(s)}(B_1) = \left[ \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{\text{y14}} \quad \mathbb{T}_1^{(s)}(B_1) = \left[ \frac{i}{2}, -\frac{i}{2}, \frac{i}{2}, -\frac{i}{2} \right]$$

$$\boxed{\text{y15}} \quad \mathbb{Q}_1^{(s)}(B_2) = \left[ \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2} \right]$$

$$\boxed{\text{y16}} \quad \mathbb{T}_1^{(s)}(B_2) = \left[ \frac{i}{2}, -\frac{i}{2}, -\frac{i}{2}, \frac{i}{2} \right]$$

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 **Site and Bond** 

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Table 5: Orbital of each site

#	site	orbital
1	<b>A</b>	$ s, \uparrow\rangle,  s, \downarrow\rangle$



Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	A	A	[1,2,3]	[s]	[s]

## Site in Unit Cell

Sites in (conventional) cell (no plus set), SL = sublattice

Table 7: 'A' (#1) site cluster (4c), 1

SL	position ( $\mathbf{s}$ )	mapping
1	[ 0.90000, 0.05000, 0.00000]	[1]
2	[ 0.10000, 0.95000, 0.00000]	[2]
3	[ 0.40000, 0.45000, 0.00000]	[3]
4	[ 0.60000, 0.55000, 0.00000]	[4]

## 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 (2a@2a), ND,  $|\mathbf{v}|=0.23324$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[ 0.20000, -0.10000, 0.00000]	[ 0.00000, 0.00000, 0.00000]	[1,-2]	(2,1)	(1,1)	[-1,1,0]
2	[ 0.20000, 0.10000, 0.00000]	[ 0.50000, 0.50000, 0.00000]	[3,-4]	(4,1)	(3,1)	[0,0,0]

Table 9: 2-th 'A'-'A' [1] (#2) bond cluster (4a@4c), D,  $|\mathbf{v}|=0.67082$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[-0.30000, -0.50000, 0.00000]	[ 0.75000, 0.80000, 0.00000]	[1]	(4,1)	(1,1)	[0,1,0]
2	[ 0.30000, 0.50000, 0.00000]	[ 0.25000, 0.20000, 0.00000]	[2]	(3,1)	(2,1)	[0,-1,0]
3	[-0.30000, 0.50000, 0.00000]	[ 0.25000, 0.70000, 0.00000]	[3]	(2,1)	(3,1)	[0,0,0]
4	[ 0.30000, -0.50000, 0.00000]	[ 0.75000, 0.30000, 0.00000]	[4]	(1,1)	(4,1)	[0,0,0]

Table 10: 3-th 'A'-'A' [1] (#3) bond cluster (4a@4c), D,  $|\mathbf{v}|=0.69311$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[-0.50000, 0.40000, 0.00000]	[ 0.65000, 0.25000, 0.00000]	[1]	(3,1)	(1,1)	[0,0,0]
2	[ 0.50000, -0.40000, 0.00000]	[ 0.35000, 0.75000, 0.00000]	[2]	(4,1)	(2,1)	[0,0,0]

*continued ...*

Table 10

SL	vector ( $\boldsymbol{v}$ )	center ( $\boldsymbol{c}$ )	mapping	head	tail	$\boldsymbol{R}$ (primitive)
3	$[-0.50000, -0.40000, 0.00000]$	$[0.15000, 0.25000, 0.00000]$	[3]	(1,1)	(3,1)	[1,0,0]
4	$[0.50000, 0.40000, 0.00000]$	$[0.85000, 0.75000, 0.00000]$	[4]	(2,1)	(4,1)	[-1,0,0]