

Model for “kappaET”

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General Condition

- Basis type: 1gs
- SAMB selection:
 - Type: [Q, G]
 - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
 - Irrep.: [A₁, A₂, B₁, B₂]
 - 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.: [A₁, A₂, B₁, B₂]
 - Spin (s): [0, 1]
- Site-cluster selection:
 - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
 - Irrep.: [A₁, A₂, B₁, B₂]
- Bond-cluster selection:
 - Type: [Q, G, M, T]
 - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
 - Irrep.: [A₁, A₂, B₁, B₂]
- Max. neighbor: 10
- Search cell range: (-2, 3), (-2, 3), (-2, 3)
- Toroidal priority: false

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):

$\mathbf{a}_1 = [1.00000, 0.00000, 0.00000]$
 $\mathbf{a}_2 = [0.00000, 1.20000, 0.00000]$
 $\mathbf{a}_3 = [0.00000, 0.00000, 1.00000]$

 — Symmetry Operation —

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	{1 0}	2	{2001 0}	3	{m010 $\frac{1}{2}\frac{1}{2}0$ }	4	{m100 $\frac{1}{2}\frac{1}{2}0$ }		

 — Harmonics —

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	-	-	$\sqrt{3}yz$

— Basis in full matrix —————

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

SAMB

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: 2a@2a

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

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

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

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

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

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

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

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

- '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: $|s, \uparrow \rangle, |s, \downarrow \rangle$

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

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

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

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

Cluster SAMB

- Site cluster

** Wyckoff: 4c

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

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

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

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

- Bond cluster

** Wyckoff: 2a@2a

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

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

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

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

** Wyckoff: 4a@4c

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

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

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

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

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

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

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

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

— Site and Bond —————

Table 5: Orbital of each site

#	site	orbital
1	A	$ 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 (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 (v)	center (c)	mapping	head	tail	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]