

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]
- 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 | $\mathbb{Q}_0(A_1)$ | A_1 | 0 | Q, T | - | - | 1 |
| 2 | $\mathbb{Q}_1(A_1)$ | A_1 | 1 | Q, T | - | - | z |
| 3 | $\mathbb{G}_2(A_1)$ | A_1 | 2 | G, M | - | - | $\sqrt{3}xy$ |
| 4 | $\mathbb{G}_0(A_2)$ | A_2 | 0 | G, M | - | - | 1 |
| 5 | $\mathbb{G}_1(A_2)$ | A_2 | 1 | G, M | - | - | z |
| 6 | $\mathbb{G}_2(A_2, 2)$ | A_2 | 2 | G, M | 2 | - | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| 7 | $\mathbb{Q}_2(A_2)$ | A_2 | 2 | Q, T | - | - | $\sqrt{3}xy$ |
| 8 | $\mathbb{G}_1(B_1)$ | B_1 | 1 | G, M | - | - | y |
| 9 | $\mathbb{Q}_1(B_1)$ | B_1 | 1 | Q, T | - | - | x |
| 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) |
|---|-------------------------------|---|-------------------------------|---|-------------------------------|---|-------------------------------|---|-----------------------------|
| 1 | $ s, \uparrow\rangle @A(1)$ | 2 | $ s, \downarrow\rangle @A(1)$ | 3 | $ s, \uparrow\rangle @A(2)$ | 4 | $ s, \downarrow\rangle @A(2)$ | 5 | $ s, \uparrow\rangle @A(3)$ |
| 6 | $ s, \downarrow\rangle @A(3)$ | 7 | $ s, \uparrow\rangle @A(4)$ | 8 | $ 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

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

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

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

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

- 'A'-'A' bond-cluster
 - * bra: $\langle s, \uparrow |, \langle s, \downarrow |$
 - * ket: $|s, \uparrow \rangle, |s, \downarrow \rangle$
 - * wyckoff: **2a@2a**

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

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

$$\boxed{\text{z4}} \quad \mathbb{Q}_2^{(c)}(A_2) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_2^{(b)}(A_2)$$

$$\boxed{\text{z14}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_1) = -\mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_1^{(b)}(B_2)$$

$$\boxed{\text{z15}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_2) = \mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_1^{(b)}(B_1)$$

$$\boxed{\text{z16}} \quad \mathbb{G}_2^{(1,-1;c)}(A_1) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_1)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_2)}{2}$$

$$\boxed{\text{z26}} \quad \mathbb{G}_0^{(1,-1;c)}(A_2) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_2)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_1)}{2}$$

$$\boxed{\text{z36}} \quad \mathbb{G}_2^{(1,-1;c)}(A_2, 2) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_2)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_1)}{2}$$

- 'A'-'A' bond-cluster
 - * bra: $\langle s, \uparrow |, \langle s, \downarrow |$
 - * ket: $|s, \uparrow \rangle, |s, \downarrow \rangle$
 - * wyckoff: **4a@4c**

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

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

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

$$\boxed{\text{z8}} \quad \mathbb{Q}_2^{(c)}(A_2) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_2^{(b)}(A_2)$$

$$\boxed{\text{z17}} \quad \mathbb{Q}_1^{(c)}(B_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_1^{(b)}(B_1)$$

$$\boxed{\text{z18}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_1) = -\mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_1^{(b)}(B_2)$$

$$\boxed{\text{z19}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_1) = \mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{M}_1^{(b)}(A_2)$$

$$\boxed{\text{z20}} \quad \mathbb{Q}_1^{(c)}(B_2) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_1^{(b)}(B_2)$$

$$\boxed{\text{z27}} \quad \mathbb{Q}_1^{(1,-1;c)}(B_2) = \mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_1^{(b)}(B_1)$$

$$\boxed{\text{z28}} \quad \mathbb{Q}_2^{(1,-1;c)}(B_2) = \mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{M}_1^{(b)}(A_2)$$

$$\boxed{\text{z29}} \quad \mathbb{G}_2^{(1,-1;c)}(A_1) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_1)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_2)}{2}$$

$$\boxed{\text{z30}} \quad \mathbb{G}_0^{(1,-1;c)}(A_2) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_2)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_1)}{2}$$

$$\boxed{\text{z37}} \quad \mathbb{G}_1^{(1,-1;c)}(A_2) = \mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_0^{(b)}(A_1)$$

$$\boxed{\text{z38}} \quad \mathbb{G}_2^{(1,-1;c)}(A_2, 2) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_1^{(b)}(B_2)}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_2)\mathbb{T}_1^{(b)}(B_1)}{2}$$

$$\boxed{\text{z39}} \quad \mathbb{G}_1^{(1,-1;c)}(B_1) = \mathbb{M}_1^{(1,-1;a)}(B_1)\mathbb{T}_0^{(b)}(A_1)$$

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

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

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

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

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

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

— 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

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

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

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

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

** Wyckoff: **4a@4c**

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

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

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

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

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

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

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

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

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] |

continued ...

Table 7

| SL | position (s) | mapping |
|----|------------------------------|---------|
| 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] |

continued ...

Table 9

| SL | vector (\mathbf{v}) | center (\mathbf{c}) | mapping | head | tail | \mathbf{R} (primitive) |
|----|------------------------------|------------------------------|---------|-------|-------|--------------------------|
| 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] |
| 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] |