Model for "C3v1"

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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.: $[A_1, A_2, E]$
  - 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.: $[A_1, A_2, E]$
  - Spin (s): `[0, 1]`
- Site-cluster selection:
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: $[A_1, A_2, E]$
- Bond-cluster selection:
  - Type: `[Q, G, M, T]`
  - Rank: `[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]`
  - Irrep.: $[A_1, A_2, E]$
- Max. neighbor: `10`
- Search cell range: `(-2, 3), (-2, 3), (-2, 3)`
- Toroidal priority: `false`

Group and Unit Cell

- Group: SG No. 156 C_{3v}^1 $P3m1$ [trigonal]
- Associated point group: PG No. 156 C_{3v} $3m$ (3m1 setting) [trigonal]
- Unit cell:
  $a=$ 1.00000, $b=$ 1.00000, $c=$ 1.00000, $\alpha=$ 90.0, $\beta=$ 90.0, $\gamma=$ 120.0
- Lattice vectors (conventional cell):
  $\boldsymbol{a}_1 =$ [1.00000, 0.00000, 0.00000]
  $\boldsymbol{a}_2 =$ [-0.50000, 0.86603, 0.00000]
  $\boldsymbol{a}_3 =$ [0.00000, 0.00000, 1.00000]

Symmetry Operation

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	$\{1\|0\}$	2	$\{3^{+}_{001}\|0\}$	3	$\{3^{-}_{001}\|0\}$	4	$\{m_{110}\|0\}$	5	$\{m_{100}\|0\}$
6	$\{m_{010}\|0\}$								

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	$\mathbb{Q}_2(A_1)$	A_1	2	Q, T	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
4	$\mathbb{G}_3(A_1)$	A_1	3	G, M	-	-	$\frac{\sqrt{10}x\left(x^2-3y^2\right)}{4}$
5	$\mathbb{Q}_3(A_1, 1)$	A_1	3	Q, T	1	-	$-\frac{z\left(3x^2+3y^2-2z^2\right)}{2}$
6	$\mathbb{Q}_3(A_1, 2)$	A_1	3	Q, T	2	-	$\frac{\sqrt{10}y\left(3x^2-y^2\right)}{4}$
7	$\mathbb{G}_0(A_2)$	A_2	0	G, M	-	-	1
8	$\mathbb{G}_1(A_2)$	A_2	1	G, M	-	-	z

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
9	$\mathbb{G}_2(A_2)$	A_2	2	$G,\ M$	-	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
10	$\mathbb{G}_3(A_2, 2)$	A_2	3	$G,\ M$	2	-	$\frac{\sqrt{10}y\left(3x^2-y^2\right)}{4}$
11	$\mathbb{Q}_3(A_2)$	A_2	3	$Q,\ T$	-	-	$\frac{\sqrt{10}x\left(x^2-3y^2\right)}{4}$
12	$\mathbb{G}_{1,1}(E)$	E	1	$G,\ M$	-	1	$-y$
13	$\mathbb{G}_{1,2}(E)$					2	x
14	$\mathbb{Q}_{1,1}(E)$	E	1	$Q,\ T$	-	1	x
15	$\mathbb{Q}_{1,2}(E)$					2	y
16	$\mathbb{G}_{2,1}(E, 2)$	E	2	$G,\ M$	2	1	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
17	$\mathbb{G}_{2,2}(E, 2)$					2	$-\sqrt{3}xy$
18	$\mathbb{Q}_{2,1}(E, 1)$	E	2	$Q,\ T$	1	1	$\sqrt{3}xz$
19	$\mathbb{Q}_{2,2}(E, 1)$					2	$\sqrt{3}yz$
20	$\mathbb{Q}_{2,1}(E, 2)$	E	2	$Q,\ T$	2	1	$\sqrt{3}xy$
21	$\mathbb{Q}_{2,2}(E, 2)$					2	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
22	$\mathbb{G}_{3,1}(E, 1)$	E	3	$G,\ M$	1	1	$\frac{\sqrt{6}y\left(x^2+y^2-4z^2\right)}{4}$
23	$\mathbb{G}_{3,2}(E, 1)$					2	$-\frac{\sqrt{6}x\left(x^2+y^2-4z^2\right)}{4}$
24	$\mathbb{G}_{3,1}(E, 2)$	E	3	$G,\ M$	2	1	$-\frac{\sqrt{15}z(x-y)(x+y)}{2}$
25	$\mathbb{G}_{3,2}(E, 2)$					2	$\sqrt{15}xyz$
26	$\mathbb{Q}_{3,1}(E, 1)$	E	3	$Q,\ T$	1	1	$-\frac{\sqrt{6}x\left(x^2+y^2-4z^2\right)}{4}$
27	$\mathbb{Q}_{3,2}(E, 1)$					2	$-\frac{\sqrt{6}y\left(x^2+y^2-4z^2\right)}{4}$
28	$\mathbb{Q}_{3,1}(E, 2)$	E	3	$Q,\ T$	2	1	$\sqrt{15}xyz$
29	$\mathbb{Q}_{3,2}(E, 2)$					2	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
30	$\mathbb{G}_{4,1}(E,2)$	E	4	$G,\ M$	2	1	$\frac{\sqrt{35}\left(x^2-2xy-y^2\right)\left(x^2+2xy-y^2\right)}{8}$
31	$\mathbb{G}_{4,2}(E,2)$					2	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$

Basis in full matrix

Table 3: dimension = 8

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

Table 4: Atomic basis (orbital part only)

orbital	definition
$\lvert p_x\rangle$	x
$\lvert p_y\rangle$	y

continued ...

Table 4

orbital	definition
$\lvert p_z\rangle$	z

SAMB

40 (all 60) SAMBs

- 'A' site-cluster
  * bra: $\langle p_x,\uparrow|$, $\langle p_x,\downarrow|$, $\langle p_y,\uparrow|$, $\langle p_y,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$
  * wyckoff: `1b`

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

$\boxed{\text{z2}}$ $\mathbb{Q}_2^{(1,-1;c)}(A_1) = \mathbb{Q}_2^{(1,-1;a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$

$\boxed{\text{z21}}$ $\mathbb{Q}_{2,1}^{(c)}(E,2) = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_0^{(s)}(A_1)}{2}$

$\boxed{\text{z22}}$ $\mathbb{Q}_{2,2}^{(c)}(E,2) = \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_0^{(s)}(A_1)}{2}$

$\boxed{\text{z23}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E,1) = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E,1)\mathbb{Q}_0^{(s)}(A_1)}{2}$

$\boxed{\text{z24}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E,1) = \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E,1)\mathbb{Q}_0^{(s)}(A_1)}{2}$

- 'B' site-cluster
  * bra: $\langle p_x,\uparrow|$, $\langle p_x,\downarrow|$, $\langle p_y,\uparrow|$, $\langle p_y,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$

* wyckoff: `1c`

$\boxed{\text{z3}}$ $\mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$

$\boxed{\text{z4}}$ $\mathbb{Q}_2^{(1,-1;c)}(A_1) = \mathbb{Q}_2^{(1,-1;a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$

$\boxed{\text{z25}}$ $\mathbb{Q}_{2,1}^{(c)}(E,2) = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_0^{(s)}(A_1)}{2}$

$\boxed{\text{z26}}$ $\mathbb{Q}_{2,2}^{(c)}(E,2) = \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_0^{(s)}(A_1)}{2}$

$\boxed{\text{z27}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E,1) = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E,1)\mathbb{Q}_0^{(s)}(A_1)}{2}$

$\boxed{\text{z28}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E,1) = \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E,1)\mathbb{Q}_0^{(s)}(A_1)}{2}$

- '`A`'-'`B`' bond-cluster
  * bra: $\langle p_x,\uparrow|$, $\langle p_x,\downarrow|$, $\langle p_y,\uparrow|$, $\langle p_y,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$
  * wyckoff: `3a@3d`

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

$\boxed{\text{z6}}$ $\mathbb{Q}_3^{(c)}(A_1,2) = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_{1,1}^{(b)}(E)}{2} + \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$

$\boxed{\text{z7}}$ $\mathbb{Q}_1^{(1,-1;c)}(A_1,a) = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E,1)\mathbb{Q}_{1,1}^{(b)}(E)}{2} + \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E,1)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$

$\boxed{\text{z8}}$ $\mathbb{Q}_1^{(1,-1;c)}(A_1,b) = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2} + \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2}$

$\boxed{\text{z9}}$ $\mathbb{Q}_2^{(1,-1;c)}(A_1) = \mathbb{Q}_2^{(1,-1;a)}(A_1)\mathbb{Q}_0^{(b)}(A_1)$

$\boxed{\text{z10}}$ $\mathbb{Q}_3^{(1,-1;c)}(A_1,1) = \dfrac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E,1)\mathbb{T}_{1,1}^{(b)}(E)}{2} + \dfrac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E,1)\mathbb{T}_{1,2}^{(b)}(E)}{2}$

$\boxed{\text{z11}}$ $$\mathbb{Q}_3^{(1,-1;c)}(A_1,2) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E,2)\mathbb{T}_{1,1}^{(b)}(E)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E,2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$\boxed{\text{z12}}$ $$\mathbb{G}_3^{(1,-1;c)}(A_1) = \mathbb{M}_3^{(1,-1;a)}(A_1)\mathbb{T}_0^{(b)}(A_1)$$

$\boxed{\text{z13}}$ $$\mathbb{Q}_3^{(c)}(A_2) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_{1,2}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$\boxed{\text{z14}}$ $$\mathbb{Q}_3^{(1,-1;c)}(A_2) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E,2)\mathbb{T}_{1,2}^{(b)}(E)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E,2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$\boxed{\text{z15}}$ $$\mathbb{G}_1^{(c)}(A_2) = \mathbb{M}_1^{(a)}(A_2)\mathbb{T}_0^{(b)}(A_1)$$

$\boxed{\text{z16}}$ $$\mathbb{G}_0^{(1,-1;c)}(A_2) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$\boxed{\text{z17}}$ $$\mathbb{G}_1^{(1,-1;c)}(A_2) = \mathbb{M}_1^{(1,-1;a)}(A_2)\mathbb{T}_0^{(b)}(A_1)$$

$\boxed{\text{z18}}$ $$\mathbb{G}_2^{(1,-1;c)}(A_2,a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E,1)\mathbb{Q}_{1,2}^{(b)}(E)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E,1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$\boxed{\text{z19}}$ $$\mathbb{G}_2^{(1,-1;c)}(A_2,b) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E,1)\mathbb{T}_{1,2}^{(b)}(E)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E,1)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$\boxed{\text{z20}}$ $$\mathbb{G}_3^{(1,-1;c)}(A_2,2) = \mathbb{M}_3^{(1,-1;a)}(A_2,2)\mathbb{T}_0^{(b)}(A_1)$$

$\boxed{\text{z29}}$ $$\mathbb{Q}_{1,1}^{(c)}(E,a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$\boxed{\text{z30}}$ $$\mathbb{Q}_{1,2}^{(c)}(E,a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$\boxed{\text{z31}}$ $$\mathbb{Q}_{1,1}^{(c)}(E,b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_{1,2}^{(b)}(E)}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$\boxed{\text{z32}}$ $$\mathbb{Q}_{1,2}^{(c)}(E,b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_{1,1}^{(b)}(E)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$\boxed{\text{z33}}$ $$\mathbb{Q}_{1,1}^{(c)}(E,c) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A_2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$\boxed{\text{z34}}$ $$\mathbb{Q}_{1,2}^{(c)}(E,c) = \frac{\sqrt{2}\mathbb{M}_{1}^{(a)}(A_2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$\boxed{\text{z35}}$ $$\mathbb{Q}_{2,1}^{(c)}(E,2) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E,2)\mathbb{Q}_{0}^{(b)}(A_1)}{2}$$

$\boxed{\text{z36}}$ $$\mathbb{Q}_{2,2}^{(c)}(E,2) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E,2)\mathbb{Q}_{0}^{(b)}(A_1)}{2}$$

$\boxed{\text{z37}}$ $$\mathbb{Q}_{1,1}^{(1,-1;c)}(E,a) = -\frac{\sqrt{2}\mathbb{Q}_{2}^{(1,-1;a)}(A_1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$\boxed{\text{z38}}$ $$\mathbb{Q}_{1,2}^{(1,-1;c)}(E,a) = -\frac{\sqrt{2}\mathbb{Q}_{2}^{(1,-1;a)}(A_1)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$\boxed{\text{z39}}$ $$\mathbb{Q}_{1,1}^{(1,-1;c)}(E,b) = -\frac{\sqrt{2}\mathbb{M}_{1}^{(1,-1;a)}(A_2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$\boxed{\text{z40}}$ $$\mathbb{Q}_{1,2}^{(1,-1;c)}(E,b) = \frac{\sqrt{2}\mathbb{M}_{1}^{(1,-1;a)}(A_2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$\boxed{\text{z41}}$ $$\mathbb{Q}_{2,1}^{(1,-1;c)}(E,1) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E,1)\mathbb{Q}_{0}^{(b)}(A_1)}{2}$$

$\boxed{\text{z42}}$ $$\mathbb{Q}_{2,2}^{(1,-1;c)}(E,1) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E,1)\mathbb{Q}_{0}^{(b)}(A_1)}{2}$$

$\boxed{\text{z43}}$ $$\mathbb{Q}_{3,1}^{(1,-1;c)}(E,1) = -\frac{\mathbb{M}_{3,1}^{(1,-1;a)}(E,2)\mathbb{T}_{1,2}^{(b)}(E)}{2} - \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(E,2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$\boxed{\text{z44}}$ $$\mathbb{Q}_{3,2}^{(1,-1;c)}(E,1) = -\frac{\mathbb{M}_{3,1}^{(1,-1;a)}(E,2)\mathbb{T}_{1,1}^{(b)}(E)}{2} + \frac{\mathbb{M}_{3,2}^{(1,-1;a)}(E,2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$\boxed{\text{z45}}$ $$\mathbb{Q}_{3,1}^{(1,-1;c)}(E,2a) = \frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(E,1)\mathbb{Q}_{1,2}^{(b)}(E)}{2} + \frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(E,1)\mathbb{Q}_{1,1}^{(b)}(E)}{2}$$

$\boxed{\text{z46}}$ $$\mathbb{Q}_{3,2}^{(1,-1;c)}(E,2a) = \frac{\mathbb{Q}_{2,1}^{(1,-1;a)}(E,1)\mathbb{Q}_{1,1}^{(b)}(E)}{2} - \frac{\mathbb{Q}_{2,2}^{(1,-1;a)}(E,1)\mathbb{Q}_{1,2}^{(b)}(E)}{2}$$

$\boxed{\text{z47}}$ $$\mathbb{Q}_{3,1}^{(1,-1;c)}(E,2b) = \frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(E,1)\mathbb{T}_{1,2}^{(b)}(E)}{8} + \frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(E,1)\mathbb{T}_{1,1}^{(b)}(E)}{8} + \frac{\sqrt{6}\mathbb{M}_{3}^{(1,-1;a)}(A_1)\mathbb{T}_{1,1}^{(b)}(E)}{8} + \frac{\sqrt{6}\mathbb{M}_{3}^{(1,-1;a)}(A_2,2)\mathbb{T}_{1,2}^{(b)}(E)}{8}$$

$\boxed{\text{z48}}$ $$\mathbb{Q}_{3,2}^{(1,-1;c)}(E,2b) = \frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(E,1)\mathbb{T}_{1,1}^{(b)}(E)}{8} - \frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(E,1)\mathbb{T}_{1,2}^{(b)}(E)}{8} + \frac{\sqrt{6}\mathbb{M}_{3}^{(1,-1;a)}(A_1)\mathbb{T}_{1,2}^{(b)}(E)}{8} - \frac{\sqrt{6}\mathbb{M}_{3}^{(1,-1;a)}(A_2,2)\mathbb{T}_{1,1}^{(b)}(E)}{8}$$

$\boxed{\text{z49}}$ $$\mathbb{G}_{1,1}^{(1,-1;c)}(E) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{0}^{(b)}(A_1)}{2}$$

$\boxed{\text{z50}}$ $$\mathbb{G}_{1,2}^{(1,-1;c)}(E) = \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_{0}^{(b)}(A_1)}{2}$$

$\boxed{\text{z51}}$ $$\mathbb{G}_{2,1}^{(1,-1;c)}(E,2a) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(E,1)\mathbb{T}_{1,2}^{(b)}(E)}{8} - \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(E,1)\mathbb{T}_{1,1}^{(b)}(E)}{8} + \frac{\sqrt{10}\mathbb{M}_{3}^{(1,-1;a)}(A_1)\mathbb{T}_{1,1}^{(b)}(E)}{8} + \frac{\sqrt{10}\mathbb{M}_{3}^{(1,-1;a)}(A_2,2)\mathbb{T}_{1,2}^{(b)}(E)}{8}$$

$\boxed{\text{z52}}$ $$\mathbb{G}_{2,2}^{(1,-1;c)}(E,2a) = -\frac{\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(E,1)\mathbb{T}_{1,1}^{(b)}(E)}{8} + \frac{\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(E,1)\mathbb{T}_{1,2}^{(b)}(E)}{8} + \frac{\sqrt{10}\mathbb{M}_{3}^{(1,-1;a)}(A_1)\mathbb{T}_{1,2}^{(b)}(E)}{8} - \frac{\sqrt{10}\mathbb{M}_{3}^{(1,-1;a)}(A_2,2)\mathbb{T}_{1,1}^{(b)}(E)}{8}$$

$\boxed{\text{z53}}$ $$\mathbb{G}_{2,1}^{(1,-1;c)}(E,2b) = \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2} + \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

$\boxed{\text{z54}}$ $$\mathbb{G}_{2,2}^{(1,-1;c)}(E,2b) = \frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E)\mathbb{T}_{1,1}^{(b)}(E)}{2} - \frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$\boxed{\text{z55}}$ $$\mathbb{G}_{3,1}^{(1,-1;c)}(E,1) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E,1)\mathbb{T}_{0}^{(b)}(A_1)}{2}$$

$\boxed{\text{z56}}$ $$\mathbb{G}_{3,2}^{(1,-1;c)}(E,1) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E,1)\mathbb{T}_{0}^{(b)}(A_1)}{2}$$

$\boxed{\text{z57}}$ $$\mathbb{G}_{3,1}^{(1,-1;c)}(E,2) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E,2)\mathbb{T}_{0}^{(b)}(A_1)}{2}$$

$\boxed{\text{z58}}$ $$\mathbb{G}_{3,2}^{(1,-1;c)}(E,2) = \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E,2)\mathbb{T}_{0}^{(b)}(A_1)}{2}$$

$\boxed{\text{z59}}$ $$\mathbb{G}_{4,1}^{(1,-1;c)}(E,2) = \frac{\mathbb{M}_{3}^{(1,-1;a)}(A_1)\mathbb{T}_{1,1}^{(b)}(E)}{2} - \frac{\mathbb{M}_{3}^{(1,-1;a)}(A_2,2)\mathbb{T}_{1,2}^{(b)}(E)}{2}$$

$\boxed{\text{z60}}$ $$\mathbb{G}_{4,2}^{(1,-1;c)}(E,2) = \frac{\mathbb{M}_{3}^{(1,-1;a)}(A_1)\mathbb{T}_{1,2}^{(b)}(E)}{2} + \frac{\mathbb{M}_{3}^{(1,-1;a)}(A_2,2)\mathbb{T}_{1,1}^{(b)}(E)}{2}$$

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

$\boxed{\text{x1}}$ $$\mathbb{Q}_{0}^{(a)}(A_1) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

$\boxed{\text{x2}}$ $$\mathbb{Q}_{2,1}^{(a)}(E,2) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x3}}$ $$\mathbb{Q}_{2,2}^{(a)}(E,2) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$$

$\boxed{\text{x4}}$ $$\mathbb{Q}_{2}^{(1,-1;a)}(A_1) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x5}}$ $$\mathbb{Q}_{2,1}^{(1,-1;a)}(E,1) = \begin{bmatrix} 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & -\frac{i}{2} & 0 \\ 0 & \frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x6}}$ $$\mathbb{Q}_{2,2}^{(1,-1;a)}(E,1) = \begin{bmatrix} 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x7}}$ $$\mathbb{M}_{1}^{(a)}(A_2) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$$

$\boxed{\text{x8}}$ $$\mathbb{M}_3^{(1,-1;a)}(A_1) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$\boxed{\text{x9}}$ $$\mathbb{M}_1^{(1,-1;a)}(A_2) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$$

$\boxed{\text{x10}}$ $$\mathbb{M}_3^{(1,-1;a)}(A_2, 2) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$\boxed{\text{x11}}$ $$\mathbb{M}_{1,1}^{(1,-1;a)}(E) = \begin{bmatrix} 0 & \frac{i}{2} & 0 & 0 \\ -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ 0 & 0 & -\frac{i}{2} & 0 \end{bmatrix}$$

$\boxed{\text{x12}}$ $$\mathbb{M}_{1,2}^{(1,-1;a)}(E) = \begin{bmatrix} 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \end{bmatrix}$$

$\boxed{\text{x13}}$ $$\mathbb{M}_{3,1}^{(1,-1;a)}(E, 1) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$$

$\boxed{\text{x14}}$ $$\mathbb{M}_{3,2}^{(1,-1;a)}(E, 1) = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} \\ -\frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 \end{bmatrix}$$

$\boxed{\text{x15}}$ $$\mathbb{M}_{3,1}^{(1,-1;a)}(E, 2) = \begin{bmatrix} -\frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$$

$\boxed{\text{x16}}$ $\mathbb{M}_{3,2}^{(1,-1;a)}(E,2) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \end{bmatrix}$

Cluster SAMB

- Site cluster

** Wyckoff: `1c`

$\boxed{\text{y1}}$ $\mathbb{Q}_{0}^{(s)}(A_1) = [1]$

** Wyckoff: `1b`

$\boxed{\text{y2}}$ $\mathbb{Q}_{0}^{(s)}(A_1) = [1]$

- Bond cluster

** Wyckoff: `3a@3d`

$\boxed{\text{y3}}$ $\mathbb{Q}_{0}^{(s)}(A_1) = \left[\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}\right]$

$\boxed{\text{y4}}$ $\mathbb{T}_{0}^{(s)}(A_1) = \left[\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}\right]$

$\boxed{\text{y5}}$ $\mathbb{Q}_{1,1}^{(s)}(E) = \left[\frac{\sqrt{2}}{2}, 0, -\frac{\sqrt{2}}{2}\right]$

$\boxed{\text{y6}}$ $\mathbb{Q}_{1,2}^{(s)}(E) = \left[-\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{3}, -\frac{\sqrt{6}}{6}\right]$

$\boxed{\text{y7}}$ $\mathbb{T}_{1,1}^{(s)}(E) = \left[\frac{\sqrt{2}i}{2}, 0, -\frac{\sqrt{2}i}{2}\right]$

$\boxed{\text{y8}}$ $\mathbb{T}_{1,2}^{(s)}(E) = \left[-\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{3}, -\frac{\sqrt{6}i}{6}\right]$

Site and Bond

Table 5: Orbital of each site

#	site	orbital
1	A	$\lvert p_x, \uparrow\rangle$, $\lvert p_x, \downarrow\rangle$, $\lvert p_y, \uparrow\rangle$, $\lvert p_y, \downarrow\rangle$
2	B	$\lvert p_x, \uparrow\rangle$, $\lvert p_x, \downarrow\rangle$, $\lvert p_y, \uparrow\rangle$, $\lvert p_y, \downarrow\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	A	B	[1]	[p]	[p]

Site in Unit Cell

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

Table 7: 'A' (#1) site cluster (1b), 3m.

SL	position (s)	mapping
1	[0.33333, 0.66667, 0.00000]	[1,2,3,4,5,6]

Table 8: 'B' (#2) site cluster (1c), 3m.

SL	position (s)	mapping
1	[0.66667, 0.33333, 0.00000]	[1,2,3,4,5,6]

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 9: 1-th 'A'-'B' [1] (#1) bond cluster (3a@3d), D, $|\boldsymbol{v}|$= 0.57735 (cartesian)

SL	vector (v)	center (c)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[-0.33333, 0.33333, 0.00000]	[0.50000, 0.50000, 0.00000]	[1,4]	(1,1)	(1,1)	[0,0,0]
2	[-0.33333,-0.66667, 0.00000]	[0.50000, 0.00000, 0.00000]	[2,6]	(1,1)	(1,1)	[0,1,0]
3	[0.66667, 0.33333, 0.00000]	[0.00000, 0.50000, 0.00000]	[3,5]	(1,1)	(1,1)	[-1,0,0]