Model for "D2h1"

Generated on 2026-02-01 15:39:45 by MultiPie 2.0.8

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_g, B_{1g}, B_{2g}, B_{3g}, A_u, B_{1u}, B_{2u}, B_{3u}]
  - 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_g, B_{1g}, B_{2g}, B_{3g}, A_u, B_{1u}, B_{2u}, B_{3u}]
  - Spin (s): [0, 1]
- Site-cluster selection:
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [A_g, B_{1g}, B_{2g}, B_{3g}, A_u, B_{1u}, B_{2u}, B_{3u}]
- Bond-cluster selection:
  - Type: [Q, G, M, T]
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [A_g, B_{1g}, B_{2g}, B_{3g}, A_u, B_{1u}, B_{2u}, B_{3u}]
- Max. neighbor: 10
- Search cell range: (-2, 3), (-2, 3), (-2, 3)
- Toroidal priority: false

Group and Unit Cell

- Group: SG No. 47 D_{2h}^{1} $Pmmm$ [orthorhombic]
- Associated point group: PG No. 47 D_{2h} mmm [orthorhombic]
- Unit cell:
  $a =$ 1.00000, $b =$ 1.20000, $c =$ 1.50000, $\alpha =$ 90.0, $\beta =$ 90.0, $\gamma =$ 90.0
- Lattice vectors (conventional cell):
  $\boldsymbol{a}_1 =$ [1.00000, 0.00000, 0.00000]
  $\boldsymbol{a}_2 =$ [0.00000, 1.20000, 0.00000]
  $\boldsymbol{a}_3 =$ [0.00000, 0.00000, 1.50000]

Symmetry Operation

Table 1: Symmetry operation

	#	SO	#	SO	#	SO	#	SO	#	SO
	1	$\{1\|0\}$	2	$\{2_{001}\|0\}$	3	$\{2_{010}\|0\}$	4	$\{2_{100}\|0\}$	5	$\{-1\|0\}$
	6	$\{\mathrm{m}_{001}\|0\}$	7	$\{\mathrm{m}_{010}\|0\}$	8	$\{\mathrm{m}_{100}\|0\}$				

Harmonics

Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A_g)$	A_g	0	Q, T	-	-	1
2	$\mathbb{Q}_2(A_g, 1)$	A_g	2	Q, T	1	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
3	$\mathbb{Q}_2(A_g, 2)$	A_g	2	Q, T	2	-	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
4	$\mathbb{G}_3(A_g)$	A_g	3	G, M	-	-	$\sqrt{15}xyz$
5	$\mathbb{G}_0(A_u)$	A_u	0	G, M	-	-	1
6	$\mathbb{G}_2(A_u, 1)$	A_u	2	G, M	1	-	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
7	$\mathbb{G}_2(A_u, 2)$	A_u	2	G, M	2	-	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
8	$\mathbb{Q}_3(A_u)$	A_u	3	Q, T	-	-	$\sqrt{15}xyz$
9	$\mathbb{G}_4(A_u, 1)$	A_u	4	G, M	1	-	$\frac{\sqrt{21}(x^4-3x^2y^2-3x^2z^2+y^4-3y^2z^2+z^4)}{6}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
10	$\mathbb{G}_1(B_{1g})$	B_{1g}	1	G, M	-	-	z
11	$\mathbb{Q}_2(B_{1g})$	B_{1g}	2	Q, T	-	-	$\sqrt{3}xy$
12	$\mathbb{G}_3(B_{1g},1)$	B_{1g}	3	G, M	1	-	$-\frac{z\left(3x^2+3y^2-2z^2\right)}{2}$
13	$\mathbb{G}_3(B_{1g},2)$	B_{1g}	3	G, M	2	-	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
14	$\mathbb{Q}_4(B_{1g},1)$	B_{1g}	4	Q, T	1	-	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
15	$\mathbb{Q}_1(B_{1u})$	B_{1u}	1	Q, T	-	-	z
16	$\mathbb{G}_2(B_{1u})$	B_{1u}	2	G, M	-	-	$\sqrt{3}xy$
17	$\mathbb{Q}_3(B_{1u},1)$	B_{1u}	3	Q, T	1	-	$-\frac{z\left(3x^2+3y^2-2z^2\right)}{2}$
18	$\mathbb{Q}_3(B_{1u},2)$	B_{1u}	3	Q, T	2	-	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
19	$\mathbb{G}_4(B_{1u},1)$	B_{1u}	4	G, M	1	-	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
20	$\mathbb{G}_1(B_{2g})$	B_{2g}	1	G, M	-	-	y
21	$\mathbb{Q}_2(B_{2g})$	B_{2g}	2	Q, T	-	-	$\sqrt{3}xz$
22	$\mathbb{G}_3(B_{2g},1)$	B_{2g}	3	G, M	1	-	$-\frac{y\left(3x^2-2y^2+3z^2\right)}{2}$
23	$\mathbb{G}_3(B_{2g},2)$	B_{2g}	3	G, M	2	-	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
24	$\mathbb{Q}_1(B_{2u})$	B_{2u}	1	Q, T	-	-	y
25	$\mathbb{G}_2(B_{2u})$	B_{2u}	2	G, M	-	-	$\sqrt{3}xz$
26	$\mathbb{Q}_3(B_{2u},1)$	B_{2u}	3	Q, T	1	-	$-\frac{y\left(3x^2-2y^2+3z^2\right)}{2}$
27	$\mathbb{Q}_3(B_{2u},2)$	B_{2u}	3	Q, T	2	-	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
28	$\mathbb{G}_1(B_{3g})$	B_{3g}	1	G, M	-	-	x
29	$\mathbb{Q}_2(B_{3g})$	B_{3g}	2	Q, T	-	-	$\sqrt{3}yz$
30	$\mathbb{G}_3(B_{3g},1)$	B_{3g}	3	G, M	1	-	$\frac{x\left(2x^2-3y^2-3z^2\right)}{2}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
31	$\mathbb{G}_3(B_{3g}, 2)$	B_{3g}	3	G, M	2	-	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
32	$\mathbb{Q}_1(B_{3u})$	B_{3u}	1	Q, T	-	-	x
33	$\mathbb{G}_2(B_{3u})$	B_{3u}	2	G, M	-	-	$\sqrt{3}yz$
34	$\mathbb{Q}_3(B_{3u}, 1)$	B_{3u}	3	Q, T	1	-	$\frac{x(2x^2-3y^2-3z^2)}{2}$
35	$\mathbb{Q}_3(B_{3u}, 2)$	B_{3u}	3	Q, T	2	-	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$

Basis in full matrix

Table 3: dimension = 8

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

Table 4: Atomic basis (orbital part only)

orbital	definition
$\|s\rangle$	1
$\|p_x\rangle$	x

continued ...

Table 4

orbital	definition
$\|p_y\rangle$	y
$\|p_z\rangle$	z

SAMB: 348 (all 348)

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

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

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

  z157 $\quad \mathbb{G}_2^{(1,-1;c)}(A_u,1) = \mathbb{G}_2^{(1,-1;a)}(A_u,1)\mathbb{Q}_0^{(s)}(A_g)$

  z158 $\quad \mathbb{G}_2^{(1,-1;c)}(A_u,2) = \mathbb{G}_2^{(1,-1;a)}(A_u,2)\mathbb{Q}_0^{(s)}(A_g)$

  z159 $\quad \mathbb{G}_0^{(1,1;c)}(A_u) = \mathbb{G}_0^{(1,1;a)}(A_u)\mathbb{Q}_0^{(s)}(A_g)$

  z210 $\quad \mathbb{Q}_1^{(c)}(B_{1u}) = \mathbb{Q}_1^{(a)}(B_{1u})\mathbb{Q}_0^{(s)}(A_g)$

  z211 $\quad \mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \mathbb{Q}_1^{(1,0;a)}(B_{1u})\mathbb{Q}_0^{(s)}(A_g)$

  z212 $\quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(s)}(A_g)$

  z259 $\quad \mathbb{Q}_1^{(c)}(B_{2u}) = \mathbb{Q}_1^{(a)}(B_{2u})\mathbb{Q}_0^{(s)}(A_g)$

z260 $\mathbb{Q}_1^{(1,0;c)}(B_{2u}) = \mathbb{Q}_1^{(1,0;a)}(B_{2u})\mathbb{Q}_0^{(s)}(A_g)$

z261 $\mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(s)}(A_g)$

z304 $\mathbb{Q}_1^{(c)}(B_{3u}) = \mathbb{Q}_1^{(a)}(B_{3u})\mathbb{Q}_0^{(s)}(A_g)$

z305 $\mathbb{Q}_1^{(1,0;c)}(B_{3u}) = \mathbb{Q}_1^{(1,0;a)}(B_{3u})\mathbb{Q}_0^{(s)}(A_g)$

z306 $\mathbb{G}_2^{(1,-1;c)}(B_{3u}) = \mathbb{G}_2^{(1,-1;a)}(B_{3u})\mathbb{Q}_0^{(s)}(A_g)$

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

  z2 $\mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(s)}(A_g)$

  z3 $\mathbb{Q}_2^{(c)}(A_g,1) = \mathbb{Q}_2^{(a)}(A_g,1)\mathbb{Q}_0^{(s)}(A_g)$

  z4 $\mathbb{Q}_2^{(c)}(A_g,2) = \mathbb{Q}_2^{(a)}(A_g,2)\mathbb{Q}_0^{(s)}(A_g)$

  z5 $\mathbb{Q}_2^{(1,-1;c)}(A_g,1) = \mathbb{Q}_2^{(1,-1;a)}(A_g,1)\mathbb{Q}_0^{(s)}(A_g)$

  z6 $\mathbb{Q}_2^{(1,-1;c)}(A_g,2) = \mathbb{Q}_2^{(1,-1;a)}(A_g,2)\mathbb{Q}_0^{(s)}(A_g)$

  z7 $\mathbb{Q}_0^{(1,1;c)}(A_g) = \mathbb{Q}_0^{(1,1;a)}(A_g)\mathbb{Q}_0^{(s)}(A_g)$

  z54 $\mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_g)$

  z55 $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_g)$

  z56 $\mathbb{G}_1^{(1,0;c)}(B_{1g}) = \mathbb{G}_1^{(1,0;a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_g)$

  z91 $\mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_g)$

  z92 $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_g)$

z93 $\mathbb{G}_1^{(1,0;c)}(B_{2g}) = \mathbb{G}_1^{(1,0;a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_g)$

z124 $\mathbb{Q}_2^{(c)}(B_{3g}) = \mathbb{Q}_2^{(a)}(B_{3g})\mathbb{Q}_0^{(s)}(A_g)$

z125 $\mathbb{Q}_2^{(1,-1;c)}(B_{3g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{3g})\mathbb{Q}_0^{(s)}(A_g)$

z126 $\mathbb{G}_1^{(1,0;c)}(B_{3g}) = \mathbb{G}_1^{(1,0;a)}(B_{3g})\mathbb{Q}_0^{(s)}(A_g)$

- `A;A_001_1` : '`A`'-'`A`' bond-cluster
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: `1c@1b`

  z8 $\mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$

  z160 $\mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})$

  z213 $\mathbb{Q}_1^{(1,-1;c)}(B_{1u}) = -\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})$

  z262 $\mathbb{Q}_1^{(1,-1;c)}(B_{2u}) = \mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$

- `A;A_001_1` : '`A`'-'`A`' bond-cluster
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
  * wyckoff: `1c@1b`

  z9 $\mathbb{Q}_0^{(c)}(A_g) = \mathbb{T}_1^{(a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})$

  z10 $\mathbb{Q}_2^{(1,-1;c)}(A_g,1) = -\mathbb{M}_2^{(1,-1;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})$

  z11 $\mathbb{Q}_0^{(1,0;c)}(A_g) = \mathbb{T}_1^{(1,0;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})$

  z57 $\mathbb{G}_2^{(1,-1;c)}(A_u,1) = \mathbb{G}_2^{(1,-1;a)}(A_u,1)\mathbb{Q}_0^{(b)}(A_g)$

  z58 $\mathbb{G}_2^{(1,-1;c)}(A_u,2) = \mathbb{G}_2^{(1,-1;a)}(A_u,2)\mathbb{Q}_0^{(b)}(A_g)$

  z59 $\mathbb{G}_0^{(1,1;c)}(A_u) = \mathbb{G}_0^{(1,1;a)}(A_u)\mathbb{Q}_0^{(b)}(A_g)$

z94 $\mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{T}_1^{(a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})$

z95 $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})$

z96 $\mathbb{Q}_2^{(1,0;c)}(B_{1g}) = \mathbb{T}_1^{(1,0;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})$

z127 $\mathbb{Q}_1^{(c)}(B_{1u}) = \mathbb{Q}_1^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$

z128 $\mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \mathbb{Q}_1^{(1,0;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$

z129 $\mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$

z161 $\mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{T}_1^{(a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{3u})$

z162 $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = -\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{3u})$

z163 $\mathbb{Q}_2^{(1,0;c)}(B_{2g}) = \mathbb{T}_1^{(1,0;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{3u})$

z214 $\mathbb{Q}_1^{(c)}(B_{2u}) = \mathbb{Q}_1^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$

z215 $\mathbb{Q}_1^{(1,0;c)}(B_{2u}) = \mathbb{Q}_1^{(1,0;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$

z216 $\mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$

z263 $\mathbb{Q}_2^{(1,-1;c)}(B_{3g}) = \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(A_u,1)\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\mathbb{M}_2^{(1,-1;a)}(A_u,2)\mathbb{T}_1^{(b)}(B_{3u})}{2}$

z264 $\mathbb{G}_1^{(1,-1;c)}(B_{3g}) = -\frac{\mathbb{M}_2^{(1,-1;a)}(A_u,1)\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(A_u,2)\mathbb{T}_1^{(b)}(B_{3u})}{2}$

z265 $\mathbb{G}_1^{(1,1;c)}(B_{3g}) = \mathbb{M}_0^{(1,1;a)}(A_u)\mathbb{T}_1^{(b)}(B_{3u})$

z307 $\mathbb{Q}_1^{(c)}(B_{3u}) = \mathbb{Q}_1^{(a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$

z308 $\mathbb{Q}_1^{(1,0;c)}(B_{3u}) = \mathbb{Q}_1^{(1,0;a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$

z309 $\mathbb{G}_2^{(1,-1;c)}(B_{3u}) = \mathbb{G}_2^{(1,-1;a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$

- `A;A_001_1` : 'A'-'A' bond-cluster
  * bra: $\langle p_x,\uparrow|$, $\langle p_x,\downarrow|$, $\langle p_y,\uparrow|$, $\langle p_y,\downarrow|$, $\langle p_z,\uparrow|$, $\langle p_z,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
  * wyckoff: `1c@1b`

z12 $\mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$

z13 $\mathbb{Q}_2^{(c)}(A_g,1) = \mathbb{Q}_2^{(a)}(A_g,1)\mathbb{Q}_0^{(b)}(A_g)$

z14 $\mathbb{Q}_2^{(c)}(A_g,2) = \mathbb{Q}_2^{(a)}(A_g,2)\mathbb{Q}_0^{(b)}(A_g)$

z15 $\mathbb{Q}_2^{(1,-1;c)}(A_g,1) = \mathbb{Q}_2^{(1,-1;a)}(A_g,1)\mathbb{Q}_0^{(b)}(A_g)$

z16 $\mathbb{Q}_2^{(1,-1;c)}(A_g,2) = \mathbb{Q}_2^{(1,-1;a)}(A_g,2)\mathbb{Q}_0^{(b)}(A_g)$

z17 $\mathbb{Q}_0^{(1,1;c)}(A_g) = \mathbb{Q}_0^{(1,1;a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$

z60 $\mathbb{Q}_3^{(1,-1;c)}(A_u) = -\mathbb{M}_3^{(1,-1;a)}(B_{3g},2)\mathbb{T}_1^{(b)}(B_{3u})$

z61 $\mathbb{Q}_3^{(1,0;c)}(A_u) = \mathbb{T}_2^{(1,0;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})$

z62 $\mathbb{G}_0^{(c)}(A_u) = \mathbb{M}_1^{(a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})$

z97 $\mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})$

z98 $\mathbb{G}_2^{(1,-1;c)}(A_u,1) = -\mathbb{M}_3^{(1,-1;a)}(B_{3g},1)\mathbb{T}_1^{(b)}(B_{3u})$

z99 $\mathbb{G}_0^{(1,1;c)}(A_u) = \mathbb{M}_1^{(1,1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})$

z130 $\mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$

z131 $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$

z132 $\mathbb{G}_1^{(1,0;c)}(B_{1g}) = \mathbb{G}_1^{(1,0;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$

z164 $\mathbb{Q}_1^{(c)}(B_{1u}) = -\mathbb{M}_1^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})$

z165 $\mathbb{Q}_1^{(1,-1;c)}(B_{1u}) = -\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})$

z166 $\mathbb{Q}_3^{(1,-1;c)}(B_{1u},1) = \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g},1)\mathbb{T}_1^{(b)}(B_{3u})}{4} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{2g},2)\mathbb{T}_1^{(b)}(B_{3u})}{4}$

z167 $\mathbb{Q}_3^{(1,-1;c)}(B_{1u},2) = \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{2g},1)\mathbb{T}_1^{(b)}(B_{3u})}{4} + \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g},2)\mathbb{T}_1^{(b)}(B_{3u})}{4}$

z168 $\mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})$

z169 $\mathbb{Q}_1^{(1,1;c)}(B_{1u}) = -\mathbb{M}_1^{(1,1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})$

z217 $\mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$

z218 $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$

z219 $\mathbb{G}_1^{(1,0;c)}(B_{2g}) = \mathbb{G}_1^{(1,0;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$

z220 $\mathbb{Q}_1^{(c)}(B_{2u}) = \mathbb{M}_1^{(a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$

z221 $\mathbb{Q}_1^{(1,-1;c)}(B_{2u}) = \mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$

z222 $\mathbb{Q}_3^{(1,-1;c)}(B_{2u},1) = -\frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g},1)\mathbb{T}_1^{(b)}(B_{3u})}{4} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{1g},2)\mathbb{T}_1^{(b)}(B_{3u})}{4}$

z266 $\mathbb{Q}_3^{(1,-1;c)}(B_{2u},2) = \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{1g},1)\mathbb{T}_1^{(b)}(B_{3u})}{4} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g},2)\mathbb{T}_1^{(b)}(B_{3u})}{4}$

z267 $\mathbb{Q}_1^{(1,0;c)}(B_{2u}) = \mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$

z268 $\mathbb{Q}_1^{(1,1;c)}(B_{2u}) = \mathbb{M}_1^{(1,1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$

z269 $\mathbb{Q}_2^{(c)}(B_{3g}) = \mathbb{Q}_2^{(a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$

z270 $\mathbb{Q}_2^{(1,-1;c)}(B_{3g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$

z271 $\mathbb{G}_1^{(1,0;c)}(B_{3g}) = \mathbb{G}_1^{(1,0;a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$

z310 $\mathbb{Q}_3^{(1,-1;c)}(B_{3u},2) = \mathbb{M}_3^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_{3u})$

z311 $\mathbb{Q}_1^{(1,0;c)}(B_{3u}) = -\frac{\mathbb{T}_2^{(1,0;a)}(A_g,1)\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(A_g,2)\mathbb{T}_1^{(b)}(B_{3u})}{2}$

z312 $\mathbb{Q}_3^{(1,0;c)}(B_{3u},2) = -\frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(A_g,1)\mathbb{T}_1^{(b)}(B_{3u})}{2} - \frac{\mathbb{T}_2^{(1,0;a)}(A_g,2)\mathbb{T}_1^{(b)}(B_{3u})}{2}$

- `A;A_002_1` : 'A'-'A' bond-cluster
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: `1b@1e`

z18 $\mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$

z170 $\mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})$

z223 $\mathbb{Q}_1^{(1,-1;c)}(B_{1u}) = \mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})$

z313 $\mathbb{Q}_1^{(1,-1;c)}(B_{3u}) = -\mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$

- `A;A_002_1` : 'A'-'A' bond-cluster
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
  * wyckoff: `1b@1e`

z19 $\mathbb{Q}_0^{(c)}(A_g) = \mathbb{T}_1^{(a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})$

z20 $\mathbb{Q}_2^{(1,-1;c)}(A_g,1) = \mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})$

z21 $\mathbb{Q}_0^{(1,0;c)}(A_g) = \mathbb{T}_1^{(1,0;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})$

z63 $\mathbb{G}_2^{(1,-1;c)}(A_u,1) = \mathbb{G}_2^{(1,-1;a)}(A_u,1)\mathbb{Q}_0^{(b)}(A_g)$

z64 $\mathbb{G}_2^{(1,-1;c)}(A_u,2) = \mathbb{G}_2^{(1,-1;a)}(A_u,2)\mathbb{Q}_0^{(b)}(A_g)$

z65 $\mathbb{G}_0^{(1,1;c)}(A_u) = \mathbb{G}_0^{(1,1;a)}(A_u)\mathbb{Q}_0^{(b)}(A_g)$

z100 $\mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{T}_1^{(a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})$

z101 $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = -\mathbb{M}_2^{(1,-1;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})$

z102 $\mathbb{Q}_2^{(1,0;c)}(B_{1g}) = \mathbb{T}_1^{(1,0;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})$

z133 $\mathbb{Q}_1^{(c)}(B_{1u}) = \mathbb{Q}_1^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$

z134 $\mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \mathbb{Q}_1^{(1,0;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$

z135 $\mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$

z171 $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(A_u,1)\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\mathbb{M}_2^{(1,-1;a)}(A_u,2)\mathbb{T}_1^{(b)}(B_{2u})}{2}$

z172 $\mathbb{G}_1^{(1,-1;c)}(B_{2g}) = -\frac{\mathbb{M}_2^{(1,-1;a)}(A_u,1)\mathbb{T}_1^{(b)}(B_{2u})}{2} - \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(A_u,2)\mathbb{T}_1^{(b)}(B_{2u})}{2}$

z173 $\mathbb{G}_1^{(1,1;c)}(B_{2g}) = \mathbb{M}_0^{(1,1;a)}(A_u)\mathbb{T}_1^{(b)}(B_{2u})$

z224 $\mathbb{Q}_1^{(c)}(B_{2u}) = \mathbb{Q}_1^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$

z225 $\mathbb{Q}_1^{(1,0;c)}(B_{2u}) = \mathbb{Q}_1^{(1,0;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$

z226 $\mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$

z272 $\mathbb{Q}_2^{(c)}(B_{3g}) = \mathbb{T}_1^{(a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{2u})$

z273 $\mathbb{Q}_2^{(1,-1;c)}(B_{3g}) = \mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{2u})$

z274 $\mathbb{Q}_2^{(1,0;c)}(B_{3g}) = \mathbb{T}_1^{(1,0;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{2u})$

z314 $\mathbb{Q}_1^{(c)}(B_{3u}) = \mathbb{Q}_1^{(a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$

z315 $\mathbb{Q}_1^{(1,0;c)}(B_{3u}) = \mathbb{Q}_1^{(1,0;a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$

z316 $\mathbb{G}_2^{(1,-1;c)}(B_{3u}) = \mathbb{G}_2^{(1,-1;a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$

- `A;A_002_1` : 'A'-'A' bond-cluster

* bra: $\langle p_x,\uparrow|$, $\langle p_x,\downarrow|$, $\langle p_y,\uparrow|$, $\langle p_y,\downarrow|$, $\langle p_z,\uparrow|$, $\langle p_z,\downarrow|$
* ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
* wyckoff: `1b@1e`

z22 $\mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$

z23 $\mathbb{Q}_2^{(c)}(A_g,1) = \mathbb{Q}_2^{(a)}(A_g,1)\mathbb{Q}_0^{(b)}(A_g)$

z24 $\mathbb{Q}_2^{(c)}(A_g,2) = \mathbb{Q}_2^{(a)}(A_g,2)\mathbb{Q}_0^{(b)}(A_g)$

z25 $\mathbb{Q}_2^{(1,-1;c)}(A_g,1) = \mathbb{Q}_2^{(1,-1;a)}(A_g,1)\mathbb{Q}_0^{(b)}(A_g)$

z26 $\mathbb{Q}_2^{(1,-1;c)}(A_g,2) = \mathbb{Q}_2^{(1,-1;a)}(A_g,2)\mathbb{Q}_0^{(b)}(A_g)$

z27 $\mathbb{Q}_0^{(1,1;c)}(A_g) = \mathbb{Q}_0^{(1,1;a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$

z66 $\mathbb{Q}_3^{(1,-1;c)}(A_u) = -\mathbb{M}_3^{(1,-1;a)}(B_{2g},2)\mathbb{T}_1^{(b)}(B_{2u})$

z67 $\mathbb{Q}_3^{(1,0;c)}(A_u) = \mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})$

z68 $\mathbb{G}_0^{(c)}(A_u) = \mathbb{M}_1^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})$

z103 $\mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})$

z104 $\mathbb{G}_2^{(1,-1;c)}(A_u,1) = -\mathbb{M}_3^{(1,-1;a)}(B_{2g},1)\mathbb{T}_1^{(b)}(B_{2u})$

z105 $\mathbb{G}_0^{(1,1;c)}(A_u) = \mathbb{M}_1^{(1,1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})$

z136 $\mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$

z137 $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$

z138 $\mathbb{G}_1^{(1,0;c)}(B_{1g}) = \mathbb{G}_1^{(1,0;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$

z174 $\mathbb{Q}_1^{(c)}(B_{1u}) = \mathbb{M}_1^{(a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})$

z175 $\mathbb{Q}_1^{(1,-1;c)}(B_{1u}) = \mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})$

z176 $\mathbb{Q}_3^{(1,-1;c)}(B_{1u},1) = -\frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{3g},1)\mathbb{T}_1^{(b)}(B_{2u})}{4} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{3g},2)\mathbb{T}_1^{(b)}(B_{2u})}{4}$

z177 $\mathbb{Q}_3^{(1,-1;c)}(B_{1u},2) = \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{3g},1)\mathbb{T}_1^{(b)}(B_{2u})}{4} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{3g},2)\mathbb{T}_1^{(b)}(B_{2u})}{4}$

z178 $\mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \mathbb{T}_2^{(1,0;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})$

z179 $\mathbb{Q}_1^{(1,1;c)}(B_{1u}) = \mathbb{M}_1^{(1,1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})$

z227 $\mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$

z228 $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$

z229 $\mathbb{G}_1^{(1,0;c)}(B_{2g}) = \mathbb{G}_1^{(1,0;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$

z230 $\mathbb{Q}_3^{(1,-1;c)}(B_{2u},2) = \mathbb{M}_3^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_{2u})$

z231 $\mathbb{Q}_1^{(1,0;c)}(B_{2u}) = -\frac{\mathbb{T}_2^{(1,0;a)}(A_g,1)\mathbb{T}_1^{(b)}(B_{2u})}{2} - \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(A_g,2)\mathbb{T}_1^{(b)}(B_{2u})}{2}$

z232 $\mathbb{Q}_3^{(1,0;c)}(B_{2u},2) = \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(A_g,1)\mathbb{T}_1^{(b)}(B_{2u})}{2} - \frac{\mathbb{T}_2^{(1,0;a)}(A_g,2)\mathbb{T}_1^{(b)}(B_{2u})}{2}$

z275 $\mathbb{Q}_2^{(c)}(B_{3g}) = \mathbb{Q}_2^{(a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$

z276 $\mathbb{Q}_2^{(1,-1;c)}(B_{3g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$

z277 $\mathbb{G}_1^{(1,0;c)}(B_{3g}) = \mathbb{G}_1^{(1,0;a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$

z317 $\mathbb{Q}_1^{(c)}(B_{3u}) = -\mathbb{M}_1^{(a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$

z318 $\mathbb{Q}_1^{(1,-1;c)}(B_{3u}) = -\mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$

z319 $\mathbb{Q}_3^{(1,-1;c)}(B_{3u},1) = \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g},1)\mathbb{T}_1^{(b)}(B_{2u})}{4} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{1g},2)\mathbb{T}_1^{(b)}(B_{2u})}{4}$

z320 $\mathbb{Q}_3^{(1,-1;c)}(B_{3u},2) = \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{1g},1)\mathbb{T}_1^{(b)}(B_{2u})}{4} + \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g},2)\mathbb{T}_1^{(b)}(B_{2u})}{4}$

z321 $\mathbb{Q}_1^{(1,0;c)}(B_{3u}) = \mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$

z322 $\mathbb{Q}_1^{(1,1;c)}(B_{3u}) = -\mathbb{M}_1^{(1,1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$

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  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
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  * wyckoff: `1a@1c`

  z28 $\mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$

  z180 $\mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{1u})$

  z278 $\mathbb{Q}_1^{(1,-1;c)}(B_{2u}) = -\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{1u})$

  z323 $\mathbb{Q}_1^{(1,-1;c)}(B_{3u}) = \mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{1u})$

- `A;A_003_1` : 'A'-'A' bond-cluster
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
  * wyckoff: `1a@1c`

  z29 $\mathbb{Q}_0^{(c)}(A_g) = \mathbb{T}_1^{(a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{1u})$

  z30 $\mathbb{Q}_2^{(1,-1;c)}(A_g,2) = \mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{1u})$

  z31 $\mathbb{Q}_0^{(1,0;c)}(A_g) = \mathbb{T}_1^{(1,0;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{1u})$

  z69 $\mathbb{G}_2^{(1,-1;c)}(A_u,1) = \mathbb{G}_2^{(1,-1;a)}(A_u,1)\mathbb{Q}_0^{(b)}(A_g)$

  z70 $\mathbb{G}_2^{(1,-1;c)}(A_u,2) = \mathbb{G}_2^{(1,-1;a)}(A_u,2)\mathbb{Q}_0^{(b)}(A_g)$

  z71 $\mathbb{G}_0^{(1,1;c)}(A_u) = \mathbb{G}_0^{(1,1;a)}(A_u)\mathbb{Q}_0^{(b)}(A_g)$

  z106 $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = -\mathbb{M}_2^{(1,-1;a)}(A_u,2)\mathbb{T}_1^{(b)}(B_{1u})$

  z107 $\mathbb{G}_1^{(1,-1;c)}(B_{1g}) = \mathbb{M}_2^{(1,-1;a)}(A_u,1)\mathbb{T}_1^{(b)}(B_{1u})$

z108 $\mathbb{G}_1^{(1,1;c)}(B_{1g}) = \mathbb{M}_0^{(1,1;a)}(A_u)\mathbb{T}_1^{(b)}(B_{1u})$

z139 $\mathbb{Q}_1^{(c)}(B_{1u}) = \mathbb{Q}_1^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$

z140 $\mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \mathbb{Q}_1^{(1,0;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$

z141 $\mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$

z181 $\mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{T}_1^{(a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{1u})$

z182 $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = \mathbb{M}_2^{(1,-1;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{1u})$

z183 $\mathbb{Q}_2^{(1,0;c)}(B_{2g}) = \mathbb{T}_1^{(1,0;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{1u})$

z233 $\mathbb{Q}_1^{(c)}(B_{2u}) = \mathbb{Q}_1^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$

z234 $\mathbb{Q}_1^{(1,0;c)}(B_{2u}) = \mathbb{Q}_1^{(1,0;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$

z235 $\mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$

z279 $\mathbb{Q}_2^{(c)}(B_{3g}) = \mathbb{T}_1^{(a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{1u})$

z280 $\mathbb{Q}_2^{(1,-1;c)}(B_{3g}) = -\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{1u})$

z281 $\mathbb{Q}_2^{(1,0;c)}(B_{3g}) = \mathbb{T}_1^{(1,0;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{1u})$

z324 $\mathbb{Q}_1^{(c)}(B_{3u}) = \mathbb{Q}_1^{(a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$

z325 $\mathbb{Q}_1^{(1,0;c)}(B_{3u}) = \mathbb{Q}_1^{(1,0;a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$

z326 $\mathbb{G}_2^{(1,-1;c)}(B_{3u}) = \mathbb{G}_2^{(1,-1;a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$

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  * bra: $\langle p_x,\uparrow|$, $\langle p_x,\downarrow|$, $\langle p_y,\uparrow|$, $\langle p_y,\downarrow|$, $\langle p_z,\uparrow|$, $\langle p_z,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
  * wyckoff: `1a@1c`

z32 $\mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$

z33 $\mathbb{Q}_2^{(c)}(A_g, 1) = \mathbb{Q}_2^{(a)}(A_g, 1)\mathbb{Q}_0^{(b)}(A_g)$

z34 $\mathbb{Q}_2^{(c)}(A_g, 2) = \mathbb{Q}_2^{(a)}(A_g, 2)\mathbb{Q}_0^{(b)}(A_g)$

z35 $\mathbb{Q}_2^{(1,-1;c)}(A_g, 1) = \mathbb{Q}_2^{(1,-1;a)}(A_g, 1)\mathbb{Q}_0^{(b)}(A_g)$

z36 $\mathbb{Q}_2^{(1,-1;c)}(A_g, 2) = \mathbb{Q}_2^{(1,-1;a)}(A_g, 2)\mathbb{Q}_0^{(b)}(A_g)$

z37 $\mathbb{Q}_0^{(1,1;c)}(A_g) = \mathbb{Q}_0^{(1,1;a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$

z72 $\mathbb{Q}_3^{(1,-1;c)}(A_u) = -\mathbb{M}_3^{(1,-1;a)}(B_{1g}, 2)\mathbb{T}_1^{(b)}(B_{1u})$

z73 $\mathbb{Q}_3^{(1,0;c)}(A_u) = \mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{1u})$

z74 $\mathbb{G}_0^{(c)}(A_u) = \mathbb{M}_1^{(a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{1u})$

z109 $\mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{1u})$

z110 $\mathbb{G}_2^{(1,-1;c)}(A_u, 1) = \mathbb{M}_3^{(1,-1;a)}(B_{1g}, 1)\mathbb{T}_1^{(b)}(B_{1u})$

z111 $\mathbb{G}_0^{(1,1;c)}(A_u) = \mathbb{M}_1^{(1,1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{1u})$

z142 $\mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$

z143 $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$

z144 $\mathbb{G}_1^{(1,0;c)}(B_{1g}) = \mathbb{G}_1^{(1,0;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$

z184 $\mathbb{Q}_3^{(1,-1;c)}(B_{1u}, 2) = \mathbb{M}_3^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_{1u})$

z185 $\mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \mathbb{T}_2^{(1,0;a)}(A_g, 1)\mathbb{T}_1^{(b)}(B_{1u})$

z186 $\mathbb{Q}_3^{(1,0;c)}(B_{1u}, 2) = \mathbb{T}_2^{(1,0;a)}(A_g, 2)\mathbb{T}_1^{(b)}(B_{1u})$

z187 $\mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$

z188 $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$

z189 $\mathbb{G}_1^{(1,0;c)}(B_{2g}) = \mathbb{G}_1^{(1,0;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$

z236 $\mathbb{Q}_1^{(c)}(B_{2u}) = -\mathbb{M}_1^{(a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{1u})$

z237 $\mathbb{Q}_1^{(1,-1;c)}(B_{2u}) = -\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{1u})$

z238 $\mathbb{Q}_3^{(1,-1;c)}(B_{2u},1) = \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{3g},1)\mathbb{T}_1^{(b)}(B_{1u})}{4} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{3g},2)\mathbb{T}_1^{(b)}(B_{1u})}{4}$

z282 $\mathbb{Q}_3^{(1,-1;c)}(B_{2u},2) = \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{3g},1)\mathbb{T}_1^{(b)}(B_{1u})}{4} + \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{3g},2)\mathbb{T}_1^{(b)}(B_{1u})}{4}$

z283 $\mathbb{Q}_1^{(1,0;c)}(B_{2u}) = \mathbb{T}_2^{(1,0;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{1u})$

z284 $\mathbb{Q}_1^{(1,1;c)}(B_{2u}) = -\mathbb{M}_1^{(1,1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{1u})$

z285 $\mathbb{Q}_2^{(c)}(B_{3g}) = \mathbb{Q}_2^{(a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$

z286 $\mathbb{Q}_2^{(1,-1;c)}(B_{3g}) = \mathbb{Q}_2^{(1,-1;a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$

z287 $\mathbb{G}_1^{(1,0;c)}(B_{3g}) = \mathbb{G}_1^{(1,0;a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$

z327 $\mathbb{Q}_1^{(c)}(B_{3u}) = \mathbb{M}_1^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{1u})$

z328 $\mathbb{Q}_1^{(1,-1;c)}(B_{3u}) = \mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{1u})$

z329 $\mathbb{Q}_3^{(1,-1;c)}(B_{3u},1) = -\frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g},1)\mathbb{T}_1^{(b)}(B_{1u})}{4} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{2g},2)\mathbb{T}_1^{(b)}(B_{1u})}{4}$

z330 $\mathbb{Q}_3^{(1,-1;c)}(B_{3u},2) = \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{2g},1)\mathbb{T}_1^{(b)}(B_{1u})}{4} - \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g},2)\mathbb{T}_1^{(b)}(B_{1u})}{4}$

z331 $\mathbb{Q}_1^{(1,0;c)}(B_{3u}) = \mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{1u})$

z332 $\mathbb{Q}_1^{(1,1;c)}(B_{3u}) = \mathbb{M}_1^{(1,1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{1u})$

- `A;A_004_1` : 'A'-'A' bond-cluster
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: `2d@1f`

  z38 $\mathbb{Q}_0^{(c)}(A_g) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$

  z75 $\mathbb{G}_0^{(1,-1;c)}(A_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$

  z190 $\mathbb{G}_2^{(1,-1;c)}(A_u,2) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$

  z191 $\mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_2^{(b)}(B_{1g})$

  z239 $\mathbb{Q}_1^{(1,-1;c)}(B_{1u}) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$

  z240 $\mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$

  z288 $\mathbb{Q}_1^{(1,-1;c)}(B_{2u}) = \mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$

  z333 $\mathbb{Q}_1^{(1,-1;c)}(B_{3u}) = -\mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$

- `A;A_004_1` : 'A'-'A' bond-cluster
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
  * wyckoff: `2d@1f`

  z39 $\mathbb{Q}_0^{(c)}(A_g) = \frac{\sqrt{2}\mathbb{T}_1^{(a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{T}_1^{(a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})}{2}$

  z40 $\mathbb{Q}_2^{(c)}(A_g,2) = -\frac{\sqrt{2}\mathbb{T}_1^{(a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{T}_1^{(a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})}{2}$

  z41 $\mathbb{Q}_2^{(1,-1;c)}(A_g,1) = \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})}{2} - \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})}{2}$

  z42 $\mathbb{Q}_2^{(1,-1;c)}(A_g,2) = -\frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})}{2} - \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})}{2}$

z43 $\mathbb{Q}_0^{(1,0;c)}(A_g) = \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})}{2}$

z44 $\mathbb{Q}_2^{(1,0;c)}(A_g, 2) = -\frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{3u})}{2}$

z76 $\mathbb{Q}_3^{(c)}(A_u) = \mathbb{Q}_1^{(a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$

z77 $\mathbb{Q}_3^{(1,0;c)}(A_u) = \mathbb{Q}_1^{(1,0;a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$

z78 $\mathbb{G}_0^{(1,-1;c)}(A_u) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$

z79 $\mathbb{G}_2^{(1,-1;c)}(A_u, 1) = \mathbb{G}_2^{(1,-1;a)}(A_u, 1)\mathbb{Q}_0^{(b)}(A_g)$

z80 $\mathbb{G}_2^{(1,-1;c)}(A_u, 2) = \mathbb{G}_2^{(1,-1;a)}(A_u, 2)\mathbb{Q}_0^{(b)}(A_g)$

z81 $\mathbb{G}_0^{(1,1;c)}(A_u) = \mathbb{G}_0^{(1,1;a)}(A_u)\mathbb{Q}_0^{(b)}(A_g)$

z112 $\mathbb{Q}_2^{(c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{T}_1^{(a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{T}_1^{(a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})}{2}$

z113 $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})}{2} - \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})}{2}$

z114 $\mathbb{Q}_2^{(1,0;c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})}{2}$

z115 $\mathbb{G}_1^{(c)}(B_{1g}) = -\frac{\sqrt{2}\mathbb{T}_1^{(a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{T}_1^{(a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})}{2}$

z116 $\mathbb{G}_1^{(1,-1;c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})}{2}$

z117 $\mathbb{G}_1^{(1,0;c)}(B_{1g}) = -\frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(B_{2u})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(B_{3u})\mathbb{T}_1^{(b)}(B_{2u})}{2}$

z145 $\mathbb{Q}_1^{(c)}(B_{1u}) = \mathbb{Q}_1^{(a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$

z146 $\mathbb{Q}_1^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_u, 2)\mathbb{Q}_2^{(b)}(B_{1g})$

z147 $\mathbb{Q}_3^{(1,-1;c)}(B_{1u},2) = -\mathbb{G}_2^{(1,-1;a)}(A_u,1)\mathbb{Q}_2^{(b)}(B_{1g})$

z148 $\mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \mathbb{Q}_1^{(1,0;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$

z149 $\mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_g)$

z150 $\mathbb{G}_2^{(1,1;c)}(B_{1u}) = \mathbb{G}_0^{(1,1;a)}(A_u)\mathbb{Q}_2^{(b)}(B_{1g})$

z192 $\mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{T}_1^{(a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{3u})$

z193 $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(A_u,1)\mathbb{T}_1^{(b)}(B_{2u})}{5} + \frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_u,2)\mathbb{T}_1^{(b)}(B_{2u})}{5} - \frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{3u})}{5}$

z194 $\mathbb{Q}_2^{(1,0;c)}(B_{2g}) = \mathbb{T}_1^{(1,0;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{3u})$

z195 $\mathbb{G}_1^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(A_u,1)\mathbb{T}_1^{(b)}(B_{2u})}{5} - \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_u,2)\mathbb{T}_1^{(b)}(B_{2u})}{10} + \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{3u})}{10}$

z196 $\mathbb{G}_3^{(1,-1;c)}(B_{2g},1) = -\frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(A_u,2)\mathbb{T}_1^{(b)}(B_{2u})}{2} - \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{3u})}{2}$

z197 $\mathbb{G}_1^{(1,1;c)}(B_{2g}) = \mathbb{M}_0^{(1,1;a)}(A_u)\mathbb{T}_1^{(b)}(B_{2u})$

z241 $\mathbb{Q}_1^{(c)}(B_{2u},a) = \mathbb{Q}_1^{(a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$

z242 $\mathbb{Q}_1^{(c)}(B_{2u},b) = \mathbb{Q}_1^{(a)}(B_{3u})\mathbb{Q}_2^{(b)}(B_{1g})$

z243 $\mathbb{Q}_1^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{3u})\mathbb{Q}_2^{(b)}(B_{1g})$

z244 $\mathbb{Q}_1^{(1,0;c)}(B_{2u},a) = \mathbb{Q}_1^{(1,0;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$

z245 $\mathbb{Q}_1^{(1,0;c)}(B_{2u},b) = \mathbb{Q}_1^{(1,0;a)}(B_{3u})\mathbb{Q}_2^{(b)}(B_{1g})$

z246 $\mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_g)$

z289 $\mathbb{Q}_2^{(c)}(B_{3g}) = \mathbb{T}_1^{(a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{2u})$

z290 $\mathbb{Q}_2^{(1,-1;c)}(B_{3g}) = \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(A_u,1)\mathbb{T}_1^{(b)}(B_{3u})}{5} + \frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_u,2)\mathbb{T}_1^{(b)}(B_{3u})}{5} + \frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{2u})}{5}$

z291 $\mathbb{Q}_2^{(1,0;c)}(B_{3g}) = \mathbb{T}_1^{(1,0;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{2u})$

z292 $\mathbb{G}_1^{(1,-1;c)}(B_{3g}) = -\frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(A_u,1)\mathbb{T}_1^{(b)}(B_{3u})}{5} + \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_u,2)\mathbb{T}_1^{(b)}(B_{3u})}{10} + \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{2u})}{10}$

z293 $\mathbb{G}_3^{(1,-1;c)}(B_{3g},1) = \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(A_u,2)\mathbb{T}_1^{(b)}(B_{3u})}{2} - \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(B_{2u})}{2}$

z294 $\mathbb{G}_1^{(1,1;c)}(B_{3g}) = \mathbb{M}_0^{(1,1;a)}(A_u)\mathbb{T}_1^{(b)}(B_{3u})$

z334 $\mathbb{Q}_1^{(c)}(B_{3u},a) = \mathbb{Q}_1^{(a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$

z335 $\mathbb{Q}_1^{(c)}(B_{3u},b) = \mathbb{Q}_1^{(a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})$

z336 $\mathbb{Q}_1^{(1,-1;c)}(B_{3u}) = -\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})$

z337 $\mathbb{Q}_1^{(1,0;c)}(B_{3u},a) = \mathbb{Q}_1^{(1,0;a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$

z338 $\mathbb{Q}_1^{(1,0;c)}(B_{3u},b) = \mathbb{Q}_1^{(1,0;a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})$

z339 $\mathbb{G}_2^{(1,-1;c)}(B_{3u}) = \mathbb{G}_2^{(1,-1;a)}(B_{3u})\mathbb{Q}_0^{(b)}(A_g)$

- `A;A_004_1` : '`A`'-'`A`' bond-cluster
  * bra: $\langle p_x,\uparrow|$, $\langle p_x,\downarrow|$, $\langle p_y,\uparrow|$, $\langle p_y,\downarrow|$, $\langle p_z,\uparrow|$, $\langle p_z,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
  * wyckoff: `2d@1f`

  z45 $\mathbb{Q}_0^{(c)}(A_g,a) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$

  z46 $\mathbb{Q}_0^{(c)}(A_g,b) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$

  z47 $\mathbb{Q}_2^{(c)}(A_g,1) = \mathbb{Q}_2^{(a)}(A_g,1)\mathbb{Q}_0^{(b)}(A_g)$

  z48 $\mathbb{Q}_2^{(c)}(A_g,2) = \mathbb{Q}_2^{(a)}(A_g,2)\mathbb{Q}_0^{(b)}(A_g)$

z49 $\mathbb{Q}_{0}^{(1,-1;c)}(A_g) = \mathbb{Q}_{2}^{(1,-1;a)}(B_{1g})\mathbb{Q}_{2}^{(b)}(B_{1g})$

z50 $\mathbb{Q}_{2}^{(1,-1;c)}(A_g,1) = \mathbb{Q}_{2}^{(1,-1;a)}(A_g,1)\mathbb{Q}_{0}^{(b)}(A_g)$

z51 $\mathbb{Q}_{2}^{(1,-1;c)}(A_g,2) = \mathbb{Q}_{2}^{(1,-1;a)}(A_g,2)\mathbb{Q}_{0}^{(b)}(A_g)$

z52 $\mathbb{Q}_{2}^{(1,0;c)}(A_g,2) = -\mathbb{G}_{1}^{(1,0;a)}(B_{1g})\mathbb{Q}_{2}^{(b)}(B_{1g})$

z53 $\mathbb{Q}_{0}^{(1,1;c)}(A_g) = \mathbb{Q}_{0}^{(1,1;a)}(A_g)\mathbb{Q}_{0}^{(b)}(A_g)$

z82 $\mathbb{Q}_{3}^{(1,-1;c)}(A_u) = -\frac{\sqrt{2}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g},2)\mathbb{T}_{1}^{(b)}(B_{2u})}{2} - \frac{\sqrt{2}\mathbb{M}_{3}^{(1,-1;a)}(B_{3g},2)\mathbb{T}_{1}^{(b)}(B_{3u})}{2}$

z83 $\mathbb{Q}_{3}^{(1,0;c)}(A_u) = \frac{\sqrt{2}\mathbb{T}_{2}^{(1,0;a)}(B_{2g})\mathbb{T}_{1}^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{T}_{2}^{(1,0;a)}(B_{3g})\mathbb{T}_{1}^{(b)}(B_{3u})}{2}$

z84 $\mathbb{G}_{0}^{(c)}(A_u) = \frac{\sqrt{2}\mathbb{M}_{1}^{(a)}(B_{2g})\mathbb{T}_{1}^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_{1}^{(a)}(B_{3g})\mathbb{T}_{1}^{(b)}(B_{3u})}{2}$

z85 $\mathbb{G}_{2}^{(c)}(A_u,2) = -\frac{\sqrt{2}\mathbb{M}_{1}^{(a)}(B_{2g})\mathbb{T}_{1}^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_{1}^{(a)}(B_{3g})\mathbb{T}_{1}^{(b)}(B_{3u})}{2}$

z86 $\mathbb{G}_{0}^{(1,-1;c)}(A_u) = \frac{\sqrt{2}\mathbb{M}_{1}^{(1,-1;a)}(B_{2g})\mathbb{T}_{1}^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_{1}^{(1,-1;a)}(B_{3g})\mathbb{T}_{1}^{(b)}(B_{3u})}{2}$

z87 $\mathbb{G}_{2}^{(1,-1;c)}(A_u,1) = -\frac{\sqrt{3}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g},1)\mathbb{T}_{1}^{(b)}(B_{2u})}{4} + \frac{\sqrt{5}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g},2)\mathbb{T}_{1}^{(b)}(B_{2u})}{4} - \frac{\sqrt{3}\mathbb{M}_{3}^{(1,-1;a)}(B_{3g},1)\mathbb{T}_{1}^{(b)}(B_{3u})}{4} - \frac{\sqrt{5}\mathbb{M}_{3}^{(1,-1;a)}(B_{3g},2)\mathbb{T}_{1}^{(b)}(B_{3u})}{4}$

z88 $\mathbb{G}_{2}^{(1,-1;c)}(A_u,2a) = -\frac{\sqrt{2}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g},1)\mathbb{T}_{1}^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_{3}^{(1,-1;a)}(B_{3g},1)\mathbb{T}_{1}^{(b)}(B_{3u})}{2}$

z89 $\mathbb{G}_{2}^{(1,-1;c)}(A_u,2b) = -\frac{\sqrt{2}\mathbb{M}_{1}^{(1,-1;a)}(B_{2g})\mathbb{T}_{1}^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_{1}^{(1,-1;a)}(B_{3g})\mathbb{T}_{1}^{(b)}(B_{3u})}{2}$

z90 $\mathbb{G}_{4}^{(1,-1;c)}(A_u,1) = \frac{\sqrt{5}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g},1)\mathbb{T}_{1}^{(b)}(B_{2u})}{4} + \frac{\sqrt{3}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g},2)\mathbb{T}_{1}^{(b)}(B_{2u})}{4} + \frac{\sqrt{5}\mathbb{M}_{3}^{(1,-1;a)}(B_{3g},1)\mathbb{T}_{1}^{(b)}(B_{3u})}{4} - \frac{\sqrt{3}\mathbb{M}_{3}^{(1,-1;a)}(B_{3g},2)\mathbb{T}_{1}^{(b)}(B_{3u})}{4}$

z118 $\mathbb{G}_{2}^{(1,0;c)}(A_u,1) = \frac{\sqrt{2}\mathbb{T}_{2}^{(1,0;a)}(B_{2g})\mathbb{T}_{1}^{(b)}(B_{2u})}{2} - \frac{\sqrt{2}\mathbb{T}_{2}^{(1,0;a)}(B_{3g})\mathbb{T}_{1}^{(b)}(B_{3u})}{2}$

z119 $\mathbb{G}_0^{(1,1;c)}(A_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$

z120 $\mathbb{G}_2^{(1,1;c)}(A_u, 2) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$

z121 $\mathbb{Q}_2^{(c)}(B_{1g}, a) = \mathbb{Q}_0^{(a)}(A_g)\mathbb{Q}_2^{(b)}(B_{1g})$

z122 $\mathbb{Q}_2^{(c)}(B_{1g}, b) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$

z123 $\mathbb{Q}_2^{(c)}(B_{1g}, c) = -\mathbb{Q}_2^{(a)}(A_g, 1)\mathbb{Q}_2^{(b)}(B_{1g})$

z151 $\mathbb{Q}_4^{(c)}(B_{1g}, 1) = \mathbb{Q}_2^{(a)}(A_g, 2)\mathbb{Q}_2^{(b)}(B_{1g})$

z152 $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}, a) = \mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$

z153 $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}, b) = -\mathbb{Q}_2^{(1,-1;a)}(A_g, 1)\mathbb{Q}_2^{(b)}(B_{1g})$

z154 $\mathbb{Q}_4^{(1,-1;c)}(B_{1g}, 1) = \mathbb{Q}_2^{(1,-1;a)}(A_g, 2)\mathbb{Q}_2^{(b)}(B_{1g})$

z155 $\mathbb{Q}_2^{(1,1;c)}(B_{1g}) = \mathbb{Q}_0^{(1,1;a)}(A_g)\mathbb{Q}_2^{(b)}(B_{1g})$

z156 $\mathbb{G}_1^{(1,0;c)}(B_{1g}) = \mathbb{G}_1^{(1,0;a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_g)$

z198 $\mathbb{Q}_1^{(c)}(B_{1u}) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$

z199 $\mathbb{Q}_1^{(1,-1;c)}(B_{1u}) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$

z200 $\mathbb{Q}_3^{(1,-1;c)}(B_{1u}, 1) = \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 1)\mathbb{T}_1^{(b)}(B_{3u})}{4} - \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 2)\mathbb{T}_1^{(b)}(B_{3u})}{4} - \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 1)\mathbb{T}_1^{(b)}(B_{2u})}{4} - \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 2)\mathbb{T}_1^{(b)}(B_{2u})}{4}$

z201 $\mathbb{Q}_3^{(1,-1;c)}(B_{1u}, 2) = \frac{\sqrt{30}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 1)\mathbb{T}_1^{(b)}(B_{3u})}{8} - \frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{2g}, 2)\mathbb{T}_1^{(b)}(B_{3u})}{8} + \frac{\sqrt{30}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 1)\mathbb{T}_1^{(b)}(B_{2u})}{8} + \frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{3g}, 2)\mathbb{T}_1^{(b)}(B_{2u})}{8}$

z202 $\mathbb{Q}_1^{(1,0;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2} + \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$

z203 $$\mathbb{Q}_3^{(1,0;c)}(B_{1u},2)=\frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2}-\frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

z204 $$\mathbb{Q}_1^{(1,1;c)}(B_{1u})=-\frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2}+\frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

z205 $$\mathbb{G}_2^{(c)}(B_{1u})=\frac{\sqrt{2}\mathbb{M}_1^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2}+\frac{\sqrt{2}\mathbb{M}_1^{(a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

z206 $$\mathbb{G}_2^{(1,-1;c)}(B_{1u},a)=-\frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{2g},1)\mathbb{T}_1^{(b)}(B_{3u})}{8}-\frac{\sqrt{30}\mathbb{M}_3^{(1,-1;a)}(B_{2g},2)\mathbb{T}_1^{(b)}(B_{3u})}{8}-\frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{3g},1)\mathbb{T}_1^{(b)}(B_{2u})}{8}+\frac{\sqrt{30}\mathbb{M}_3^{(1,-1;a)}(B_{3g},2)\mathbb{T}_1^{(b)}(B_{2u})}{8}$$

z207 $$\mathbb{G}_2^{(1,-1;c)}(B_{1u},b)=\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2}+\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

z208 $$\mathbb{G}_4^{(1,-1;c)}(B_{1u},1)=-\frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{2g},1)\mathbb{T}_1^{(b)}(B_{3u})}{4}-\frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{2g},2)\mathbb{T}_1^{(b)}(B_{3u})}{4}+\frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{3g},1)\mathbb{T}_1^{(b)}(B_{2u})}{4}-\frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{3g},2)\mathbb{T}_1^{(b)}(B_{2u})}{4}$$

z209 $$\mathbb{G}_2^{(1,1;c)}(B_{1u})=\frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{3u})}{2}+\frac{\sqrt{2}\mathbb{M}_1^{(1,1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{2u})}{2}$$

z247 $$\mathbb{Q}_2^{(c)}(B_{2g},a)=\mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$$

z248 $$\mathbb{Q}_2^{(c)}(B_{2g},b)=\mathbb{Q}_2^{(a)}(B_{3g})\mathbb{Q}_2^{(b)}(B_{1g})$$

z249 $$\mathbb{Q}_2^{(1,-1;c)}(B_{2g},a)=\mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$$

z250 $$\mathbb{Q}_2^{(1,-1;c)}(B_{2g},b)=\mathbb{Q}_2^{(1,-1;a)}(B_{3g})\mathbb{Q}_2^{(b)}(B_{1g})$$

z251 $$\mathbb{Q}_2^{(1,0;c)}(B_{2g})=\mathbb{G}_1^{(1,0;a)}(B_{3g})\mathbb{Q}_2^{(b)}(B_{1g})$$

z252 $$\mathbb{G}_1^{(1,0;c)}(B_{2g})=\mathbb{G}_1^{(1,0;a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_g)$$

z253 $$\mathbb{Q}_1^{(c)}(B_{2u})=\mathbb{M}_1^{(a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$$

z254 $$\mathbb{Q}_1^{(1,-1;c)}(B_{2u})=\mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$$

z255 $$\mathbb{Q}_3^{(1,-1;c)}(B_{2u},1)=-\frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g},1)\mathbb{T}_1^{(b)}(B_{3u})}{4}-\frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{1g},2)\mathbb{T}_1^{(b)}(B_{3u})}{4}$$

z256 $\mathbb{Q}_3^{(1,-1;c)}(B_{2u},2) = \frac{2\sqrt{22}\mathbb{M}_3^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_{2u})}{11} + \frac{\sqrt{330}\mathbb{M}_3^{(1,-1;a)}(B_{1g},1)\mathbb{T}_1^{(b)}(B_{3u})}{44} - \frac{3\sqrt{22}\mathbb{M}_3^{(1,-1;a)}(B_{1g},2)\mathbb{T}_1^{(b)}(B_{3u})}{44}$

z257 $\mathbb{Q}_1^{(1,0;c)}(B_{2u}) = -\frac{\sqrt{7}\mathbb{T}_2^{(1,0;a)}(A_g,1)\mathbb{T}_1^{(b)}(B_{2u})}{7} - \frac{\sqrt{21}\mathbb{T}_2^{(1,0;a)}(A_g,2)\mathbb{T}_1^{(b)}(B_{2u})}{7} + \frac{\sqrt{21}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})}{7}$

z258 $\mathbb{Q}_3^{(1,0;c)}(B_{2u},1) = -\frac{\sqrt{21}\mathbb{T}_2^{(1,0;a)}(A_g,1)\mathbb{T}_1^{(b)}(B_{2u})}{14} - \frac{3\sqrt{7}\mathbb{T}_2^{(1,0;a)}(A_g,2)\mathbb{T}_1^{(b)}(B_{2u})}{14} - \frac{2\sqrt{7}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})}{7}$

z295 $\mathbb{Q}_3^{(1,0;c)}(B_{2u},2) = \frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(A_g,1)\mathbb{T}_1^{(b)}(B_{2u})}{2} - \frac{\mathbb{T}_2^{(1,0;a)}(A_g,2)\mathbb{T}_1^{(b)}(B_{2u})}{2}$

z296 $\mathbb{Q}_1^{(1,1;c)}(B_{2u}) = \mathbb{M}_1^{(1,1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{3u})$

z297 $\mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{33}\mathbb{M}_3^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_{2u})}{11} - \frac{\sqrt{55}\mathbb{M}_3^{(1,-1;a)}(B_{1g},1)\mathbb{T}_1^{(b)}(B_{3u})}{11} + \frac{\sqrt{33}\mathbb{M}_3^{(1,-1;a)}(B_{1g},2)\mathbb{T}_1^{(b)}(B_{3u})}{11}$

z298 $\mathbb{Q}_2^{(c)}(B_{3g},a) = \mathbb{Q}_2^{(a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$

z299 $\mathbb{Q}_2^{(c)}(B_{3g},b) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$

z300 $\mathbb{Q}_2^{(1,-1;c)}(B_{3g},a) = \mathbb{Q}_2^{(1,-1;a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$

z301 $\mathbb{Q}_2^{(1,-1;c)}(B_{3g},b) = \mathbb{Q}_2^{(1,-1;a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$

z302 $\mathbb{Q}_2^{(1,0;c)}(B_{3g}) = -\mathbb{G}_1^{(1,0;a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$

z303 $\mathbb{G}_1^{(1,0;c)}(B_{3g}) = \mathbb{G}_1^{(1,0;a)}(B_{3g})\mathbb{Q}_0^{(b)}(A_g)$

z340 $\mathbb{Q}_1^{(c)}(B_{3u}) = -\mathbb{M}_1^{(a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$

z341 $\mathbb{Q}_1^{(1,-1;c)}(B_{3u}) = -\mathbb{M}_1^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$

z342 $\mathbb{Q}_3^{(1,-1;c)}(B_{3u},1) = \frac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g},1)\mathbb{T}_1^{(b)}(B_{2u})}{4} - \frac{\sqrt{10}\mathbb{M}_3^{(1,-1;a)}(B_{1g},2)\mathbb{T}_1^{(b)}(B_{2u})}{4}$

z343 $\mathbb{Q}_3^{(1,-1;c)}(B_{3u},2) = \frac{2\sqrt{22}\mathbb{M}_3^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_{3u})}{11} + \frac{\sqrt{330}\mathbb{M}_3^{(1,-1;a)}(B_{1g},1)\mathbb{T}_1^{(b)}(B_{2u})}{44} + \frac{3\sqrt{22}\mathbb{M}_3^{(1,-1;a)}(B_{1g},2)\mathbb{T}_1^{(b)}(B_{2u})}{44}$

z344 $\mathbb{Q}_1^{(1,0;c)}(B_{3u}) = -\frac{\sqrt{7}\mathbb{T}_2^{(1,0;a)}(A_g,1)\mathbb{T}_1^{(b)}(B_{3u})}{7} + \frac{\sqrt{21}\mathbb{T}_2^{(1,0;a)}(A_g,2)\mathbb{T}_1^{(b)}(B_{3u})}{7} + \frac{\sqrt{21}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})}{7}$

z345 $\mathbb{Q}_3^{(1,0;c)}(B_{3u},1) = -\frac{\sqrt{21}\mathbb{T}_2^{(1,0;a)}(A_g,1)\mathbb{T}_1^{(b)}(B_{3u})}{14} + \frac{3\sqrt{7}\mathbb{T}_2^{(1,0;a)}(A_g,2)\mathbb{T}_1^{(b)}(B_{3u})}{14} - \frac{2\sqrt{7}\mathbb{T}_2^{(1,0;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})}{7}$

z346 $\mathbb{Q}_3^{(1,0;c)}(B_{3u},2) = -\frac{\sqrt{3}\mathbb{T}_2^{(1,0;a)}(A_g,1)\mathbb{T}_1^{(b)}(B_{3u})}{2} - \frac{\mathbb{T}_2^{(1,0;a)}(A_g,2)\mathbb{T}_1^{(b)}(B_{3u})}{2}$

z347 $\mathbb{Q}_1^{(1,1;c)}(B_{3u}) = -\mathbb{M}_1^{(1,1;a)}(B_{1g})\mathbb{T}_1^{(b)}(B_{2u})$

z348 $\mathbb{G}_2^{(1,-1;c)}(B_{3u}) = \frac{\sqrt{33}\mathbb{M}_3^{(1,-1;a)}(A_g)\mathbb{T}_1^{(b)}(B_{3u})}{11} - \frac{\sqrt{55}\mathbb{M}_3^{(1,-1;a)}(B_{1g},1)\mathbb{T}_1^{(b)}(B_{2u})}{11} - \frac{\sqrt{33}\mathbb{M}_3^{(1,-1;a)}(B_{1g},2)\mathbb{T}_1^{(b)}(B_{2u})}{11}$

Atomic SAMB

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

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

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

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

x4 $\mathbb{M}_1^{(1,-1;a)}(B_{3g}) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$

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

x5 $\mathbb{Q}_1^{(a)}(B_{1u}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$

x6 $\mathbb{Q}_1^{(a)}(B_{2u}) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$

x7 $\mathbb{Q}_1^{(a)}(B_{3u}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$

x8 $\mathbb{Q}_1^{(1,0;a)}(B_{1u}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$

x9 $\mathbb{Q}_1^{(1,0;a)}(B_{2u}) = \begin{bmatrix} \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$

x10 $\mathbb{Q}_1^{(1,0;a)}(B_{3u}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$

x11 $\mathbb{G}_2^{(1,-1;a)}(A_u, 1) = \begin{bmatrix} 0 & -\frac{\sqrt{6}i}{12} & 0 & -\frac{\sqrt{6}}{12} & \frac{\sqrt{6}i}{6} & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}i}{6} \end{bmatrix}$

x12 $\mathbb{G}_2^{(1,-1;a)}(A_u, 2) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$

x13 $\mathbb{G}_2^{(1,-1;a)}(B_{1u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$

x14 $\mathbb{G}_2^{(1,-1;a)}(B_{2u}) = \begin{bmatrix} \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$

x15 $\mathbb{G}_2^{(1,-1;a)}(B_{3u}) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$

x16 $\mathbb{G}_0^{(1,1;a)}(A_u) = \begin{bmatrix} 0 & \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \end{bmatrix}$

x17 $\mathbb{M}_2^{(1,-1;a)}(A_u, 1) = \begin{bmatrix} 0 & -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}}{6} & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{6}}{6} \end{bmatrix}$

x18 $\mathbb{M}_2^{(1,-1;a)}(A_u, 2) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ \frac{\sqrt{2}}{4} & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$

x19 $\mathbb{M}_2^{(1,-1;a)}(B_{1u}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$

x20 $\mathbb{M}_2^{(1,-1;a)}(B_{2u}) = \begin{bmatrix} \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \end{bmatrix}$

x21 $\mathbb{M}_2^{(1,-1;a)}(B_{3u}) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$

x22 $\mathbb{M}_0^{(1,1;a)}(A_u) = \begin{bmatrix} 0 & \frac{\sqrt{3}}{6} & 0 & -\frac{\sqrt{3}i}{6} & \frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} \end{bmatrix}$

x23 $\mathbb{T}_1^{(a)}(B_{1u}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} \end{bmatrix}$

x24 $\mathbb{T}_1^{(a)}(B_{2u}) = \begin{bmatrix} 0 & 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$

x25 $\mathbb{T}_1^{(a)}(B_{3u}) = \begin{bmatrix} \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$

x26 $\mathbb{T}_1^{(1,0;a)}(B_{1u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$

x27 $\mathbb{T}_1^{(1,0;a)}(B_{2u}) = \begin{bmatrix} \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \end{bmatrix}$

x28 $\mathbb{T}_1^{(1,0;a)}(B_{3u}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & \frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$

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

x29 $\mathbb{Q}_0^{(a)}(A_g) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \end{bmatrix}$

x30 $\mathbb{Q}_2^{(a)}(A_g,1) = \begin{bmatrix} -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$

x31 $\mathbb{Q}_2^{(a)}(A_g,2) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$

x32 $\mathbb{Q}_2^{(a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$

x33 $\mathbb{Q}_2^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$

x34 $\mathbb{Q}_2^{(a)}(B_{3g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$

x35 $\mathbb{Q}_2^{(1,-1;a)}(A_g, 1) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & \frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{12} \\ 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & \frac{\sqrt{6}i}{12} & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{bmatrix}$

x36 $\mathbb{Q}_2^{(1,-1;a)}(A_g,2) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \end{bmatrix}$

x37 $\mathbb{Q}_2^{(1,-1;a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$

x38 $\mathbb{Q}_2^{(1,-1;a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{bmatrix}$

x39 $\mathbb{Q}_2^{(1,-1;a)}(B_{3g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{bmatrix}$

x40 $\mathbb{Q}_0^{(1,1;a)}(A_g) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ \frac{\sqrt{3}i}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{bmatrix}$

x41 $\mathbb{G}_1^{(1,0;a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$

x42 $\mathbb{G}_1^{(1,0;a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & \frac{\sqrt{2}i}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 \end{bmatrix}$

x43 $\mathbb{G}_1^{(1,0;a)}(B_{3g}) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{2}}{4} & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 \\ -\frac{\sqrt{2}}{4} & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{2}i}{4} & 0 & 0 & 0 & 0 \end{bmatrix}$

x44 $\mathbb{M}_1^{(a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$

x45 $\mathbb{M}_1^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{i}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{i}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$

x46 $\mathbb{M}_1^{(a)}(B_{3g}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & \frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$

x47 $\mathbb{M}_3^{(1,-1;a)}(A_g) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \\ \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \end{bmatrix}$

x48 $\mathbb{M}_1^{(1,-1;a)}(B_{1g}) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \end{bmatrix}$

x49 $\mathbb{M}_3^{(1,-1;a)}(B_{1g},1) = \begin{bmatrix} -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 \\ 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & \frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{5}}{10} & -\frac{\sqrt{5}i}{10} & 0 \\ 0 & -\frac{\sqrt{5}}{10} & 0 & \frac{\sqrt{5}i}{10} & \frac{\sqrt{5}}{5} & 0 \\ -\frac{\sqrt{5}}{10} & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & -\frac{\sqrt{5}}{5} \end{bmatrix}$

x50 $\mathbb{M}_3^{(1,-1;a)}(B_{1g},2) = \begin{bmatrix} \frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & \frac{\sqrt{3}}{6} & -\frac{\sqrt{3}i}{6} & 0 \\ 0 & \frac{\sqrt{3}}{6} & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 \\ \frac{\sqrt{3}}{6} & 0 & -\frac{\sqrt{3}i}{6} & 0 & 0 & 0 \end{bmatrix}$

x51 $\mathbb{M}_1^{(1,-1;a)}(B_{2g}) = \begin{bmatrix} 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}i}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}i}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$

x52 $\mathbb{M}_3^{(1,-1;a)}(B_{2g},1) = \begin{bmatrix} 0 & \frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 \\ -\frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{5}}{10} & 0 & -\frac{\sqrt{5}i}{5} & -\frac{\sqrt{5}}{10} & 0 \\ -\frac{\sqrt{5}}{10} & 0 & \frac{\sqrt{5}i}{5} & 0 & 0 & \frac{\sqrt{5}}{10} \\ 0 & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & \frac{\sqrt{5}i}{10} \\ 0 & 0 & 0 & \frac{\sqrt{5}}{10} & -\frac{\sqrt{5}i}{10} & 0 \end{bmatrix}$

x53 $\mathbb{M}_3^{(1,-1;a)}(B_{2g},2) = \begin{bmatrix} 0 & \frac{\sqrt{3}i}{6} & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 \\ -\frac{\sqrt{3}i}{6} & 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{6} & 0 & 0 & \frac{\sqrt{3}}{6} & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} \\ 0 & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}i}{6} \\ 0 & 0 & 0 & -\frac{\sqrt{3}}{6} & \frac{\sqrt{3}i}{6} & 0 \end{bmatrix}$

x54 $\mathbb{M}_1^{(1,-1;a)}(B_{3g}) = \begin{bmatrix} 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{6} & 0 \end{bmatrix}$

x55 $\mathbb{M}_3^{(1,-1;a)}(B_{3g},1) = \begin{bmatrix} 0 & \frac{\sqrt{5}}{5} & 0 & \frac{\sqrt{5}i}{10} & -\frac{\sqrt{5}}{10} & 0 \\ \frac{\sqrt{5}}{5} & 0 & -\frac{\sqrt{5}i}{10} & 0 & 0 & \frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 \\ -\frac{\sqrt{5}i}{10} & 0 & -\frac{\sqrt{5}}{10} & 0 & 0 & 0 \\ -\frac{\sqrt{5}}{10} & 0 & 0 & 0 & 0 & -\frac{\sqrt{5}}{10} \\ 0 & \frac{\sqrt{5}}{10} & 0 & 0 & -\frac{\sqrt{5}}{10} & 0 \end{bmatrix}$

x56 $\mathbb{M}_3^{(1,-1;a)}(B_{3g},2) = \begin{bmatrix} 0 & 0 & 0 & -\frac{\sqrt{3}i}{6} & -\frac{\sqrt{3}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{3}i}{6} & 0 & 0 & \frac{\sqrt{3}}{6} \\ 0 & -\frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 \\ \frac{\sqrt{3}i}{6} & 0 & \frac{\sqrt{3}}{6} & 0 & 0 & 0 \\ -\frac{\sqrt{3}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{6} \\ 0 & \frac{\sqrt{3}}{6} & 0 & 0 & -\frac{\sqrt{3}}{6} & 0 \end{bmatrix}$

x57 $\mathbb{M}_1^{(1,1;a)}(B_{1g}) = \begin{bmatrix} -\frac{\sqrt{30}}{30} & 0 & 0 & 0 & 0 & \frac{\sqrt{30}}{20} \\ 0 & \frac{\sqrt{30}}{30} & 0 & 0 & \frac{\sqrt{30}}{20} & 0 \\ 0 & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 & -\frac{\sqrt{30}i}{20} \\ 0 & 0 & 0 & \frac{\sqrt{30}}{30} & \frac{\sqrt{30}i}{20} & 0 \\ 0 & \frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{20} & \frac{\sqrt{30}}{15} & 0 \\ \frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{20} & 0 & 0 & -\frac{\sqrt{30}}{15} \end{bmatrix}$

x58 $\mathbb{M}_1^{(1,1;a)}(B_{2g}) = \begin{bmatrix} 0 & \frac{\sqrt{30}i}{30} & 0 & \frac{\sqrt{30}}{20} & 0 & 0 \\ -\frac{\sqrt{30}i}{30} & 0 & \frac{\sqrt{30}}{20} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{30}}{20} & 0 & -\frac{\sqrt{30}i}{15} & \frac{\sqrt{30}}{20} & 0 \\ \frac{\sqrt{30}}{20} & 0 & \frac{\sqrt{30}i}{15} & 0 & 0 & -\frac{\sqrt{30}}{20} \\ 0 & 0 & \frac{\sqrt{30}}{20} & 0 & 0 & \frac{\sqrt{30}i}{30} \\ 0 & 0 & 0 & -\frac{\sqrt{30}}{20} & -\frac{\sqrt{30}i}{30} & 0 \end{bmatrix}$

x59 $\mathbb{M}_1^{(1,1;a)}(B_{3g}) = \begin{bmatrix} 0 & \frac{\sqrt{30}}{15} & 0 & -\frac{\sqrt{30}i}{20} & \frac{\sqrt{30}}{20} & 0 \\ \frac{\sqrt{30}}{15} & 0 & \frac{\sqrt{30}i}{20} & 0 & 0 & -\frac{\sqrt{30}}{20} \\ 0 & -\frac{\sqrt{30}i}{20} & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 \\ \frac{\sqrt{30}i}{20} & 0 & -\frac{\sqrt{30}}{30} & 0 & 0 & 0 \\ \frac{\sqrt{30}}{20} & 0 & 0 & 0 & 0 & -\frac{\sqrt{30}}{30} \\ 0 & -\frac{\sqrt{30}}{20} & 0 & 0 & -\frac{\sqrt{30}}{30} & 0 \end{bmatrix}$

x60 $\mathbb{T}_2^{(1,0;a)}(A_g,1) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}i}{4} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{2}i}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{2}}{4} & 0 \\ 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 & 0 & 0 \end{bmatrix}$

x61 $\mathbb{T}_2^{(1,0;a)}(A_g,2) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ -\frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}}{6} & 0 & 0 & \frac{\sqrt{6}}{12} & 0 \\ 0 & -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 \\ \frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \end{bmatrix}$

x62 $\mathbb{T}_2^{(1,0;a)}(B_{1g}) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ 0 & -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{bmatrix}$

x63 $\mathbb{T}_2^{(1,0;a)}(B_{2g}) = \begin{bmatrix} 0 & \frac{\sqrt{6}i}{6} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 \\ -\frac{\sqrt{6}i}{6} & 0 & \frac{\sqrt{6}}{12} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & 0 & \frac{\sqrt{6}}{12} \\ 0 & 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}i}{6} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{12} & \frac{\sqrt{6}i}{6} & 0 \end{bmatrix}$

x64 $\mathbb{T}_2^{(1,0;a)}(B_{3g}) = \begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \end{bmatrix}$

Cluster SAMB

- Site cluster

** Wyckoff: `1a`

y1 $\mathbb{Q}_0^{(s)}(A_g) = [1]$

- Bond cluster

** Wyckoff: `1b@1e`

y2 $\mathbb{Q}_0^{(s)}(A_g) = [1]$

y3 $\mathbb{T}_1^{(s)}(B_{2u}) = [i]$

** Wyckoff: `1c@1b`

y4 $\mathbb{Q}_0^{(s)}(A_g) = [1]$

y5 $\mathbb{T}_1^{(s)}(B_{3u}) = [i]$

** Wyckoff: `1a@1c`

y6 $\mathbb{Q}_0^{(s)}(A_g) = [1]$

y7 $\mathbb{T}_1^{(s)}(B_{1u}) = [i]$

** Wyckoff: `2d@1f`

y8 $\mathbb{Q}_0^{(s)}(A_g) = \left[\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right]$

y9 $\mathbb{Q}_2^{(s)}(B_{1g}) = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}\right]$

y10 $\mathbb{T}_1^{(s)}(B_{2u}) = \left[\frac{\sqrt{2}i}{2}, \frac{\sqrt{2}i}{2}\right]$

y11 $\mathbb{T}_1^{(s)}(B_{3u}) = \left[\frac{\sqrt{2}i}{2}, -\frac{\sqrt{2}i}{2}\right]$

Site and Bond

Table 5: Orbital of each site

#	site	orbital
1	`A`	$\|s,\uparrow\rangle$, $\|s,\downarrow\rangle$, $\|p_x,\uparrow\rangle$, $\|p_x,\downarrow\rangle$, $\|p_y,\uparrow\rangle$, $\|p_y,\downarrow\rangle$, $\|p_z,\uparrow\rangle$, $\|p_z,\downarrow\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	`A`	`A`	`[1,2,3,4]`	`[s,p]`	`[s,p]`

Site in Unit Cell

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

Table 7: 'A' (#1) site cluster (1a), mmm

SL	position ($\boldsymbol{s}$)	mapping
1	[0.00000, 0.00000, 0.00000]	[1,2,3,4,5,6,7,8]

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 (1c@1b), ND, $|\boldsymbol{v}|$= 1.0 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[-1.00000, 0.00000, 0.00000]	[0.50000, 0.00000, 0.00000]	[1,-2,-3,4,-5,6,7,-8]	(1,1)	(1,1)	[1,0,0]

Table 9: 2-th 'A'-'A' [1] (#2) bond cluster (1b@1e), ND, $|\boldsymbol{v}|$= 1.2 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[0.00000,-1.00000, 0.00000]	[0.00000, 0.50000, 0.00000]	[1,-2,3,-4,-5,6,-7,8]	(1,1)	(1,1)	[0,1,0]

Table 10: 3-th 'A'-'A' [1] (#3) bond cluster (1a@1c), ND, $|\boldsymbol{v}|$= 1.5 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[0.00000, 0.00000,-1.00000]	[0.00000, 0.00000, 0.50000]	[1,2,-3,-4,-5,-6,7,8]	(1,1)	(1,1)	[0,0,1]

Table 11: 4-th 'A'-'A' [1] (#4) bond cluster (2d@1f), ND, $|\boldsymbol{v}|$= 1.56205 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[-1.00000,-1.00000, 0.00000]	[0.50000, 0.50000, 0.00000]	[1,-2,-5,6]	(1,1)	(1,1)	[1,1,0]
2	[1.00000,-1.00000, 0.00000]	[0.50000, 0.50000, 0.00000]	[3,-4,-7,8]	(1,1)	(1,1)	[-1,1,0]