Model for "BCT"

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

Group and Unit Cell

- Group: SG No. 139 D_{4h}^{17} $I4/mmm$ [tetragonal]
- Associated point group: PG No. 139 D_{4h} $4/mmm$ [tetragonal]
- Unit cell:
  $a =$ 1.00000, $b =$ 1.00000, $c =$ 2.32000, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 90.0$
- Lattice vectors (conventional cell):
  $\boldsymbol{a}_1 =$ [1.00000, 0.00000, 0.00000]
  $\boldsymbol{a}_2 =$ [0.00000, 1.00000, 0.00000]
  $\boldsymbol{a}_3 =$ [0.00000, 0.00000, 2.32000]

- Plus sets:
  $+[0,\,0,\,0],\quad +\left[\frac{1}{2},\,\frac{1}{2},\,\frac{1}{2}\right]$

Symmetry Operation

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	$\{1\|0\}$	2	$\{2_{001}\|0\}$	3	$\{4^{+}_{001}\|0\}$	4	$\{4^{-}_{001}\|0\}$	5	$\{2_{010}\|0\}$
6	$\{2_{100}\|0\}$	7	$\{2_{110}\|0\}$	8	$\{2_{1-10}\|0\}$	9	$\{-1\|0\}$	10	$\{m_{001}\|0\}$
11	$\{-4^{+}_{001}\|0\}$	12	$\{-4^{-}_{001}\|0\}$	13	$\{m_{010}\|0\}$	14	$\{m_{100}\|0\}$	15	$\{m_{110}\|0\}$
16	$\{m_{1-10}\|0\}$								

Harmonics

Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A_{1g})$	A_{1g}	0	$Q,\,T$	-	-	1
2	$\mathbb{Q}_2(A_{1g})$	A_{1g}	2	$Q,\,T$	-	-	$-\frac{x^2}{2}-\frac{y^2}{2}+z^2$
3	$\mathbb{G}_0(A_{1u})$	A_{1u}	0	$G,\,M$	-	-	1
4	$\mathbb{G}_2(A_{1u})$	A_{1u}	2	$G,\,M$	-	-	$-\frac{x^2}{2}-\frac{y^2}{2}+z^2$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
5	$\mathbb{G}_4(A_{1u},1)$	A_{1u}	4	$G,\ M$	1	-	$\frac{\sqrt{21}\left(x^4-3x^2y^2-3x^2z^2+y^4-3y^2z^2+z^4\right)}{6}$
6	$\mathbb{Q}_5(A_{1u})$	A_{1u}	5	$Q,\ T$	-	-	$\frac{3\sqrt{35}xyz(x-y)(x+y)}{2}$
7	$\mathbb{G}_1(A_{2g})$	A_{2g}	1	$G,\ M$	-	-	z
8	$\mathbb{G}_3(A_{2g})$	A_{2g}	3	$G,\ M$	-	-	$-\frac{z\left(3x^2+3y^2-2z^2\right)}{2}$
9	$\mathbb{Q}_4(A_{2g})$	A_{2g}	4	$Q,\ T$	-	-	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
10	$\mathbb{Q}_1(A_{2u})$	A_{2u}	1	$Q,\ T$	-	-	z
11	$\mathbb{Q}_3(A_{2u})$	A_{2u}	3	$Q,\ T$	-	-	$-\frac{z\left(3x^2+3y^2-2z^2\right)}{2}$
12	$\mathbb{G}_4(A_{2u})$	A_{2u}	4	$G,\ M$	-	-	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
13	$\mathbb{Q}_2(B_{1g})$	B_{1g}	2	$Q,\ T$	-	-	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
14	$\mathbb{G}_3(B_{1g})$	B_{1g}	3	$G,\ M$	-	-	$\sqrt{15}xyz$
15	$\mathbb{G}_2(B_{1u})$	B_{1u}	2	$G,\ M$	-	-	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
16	$\mathbb{Q}_3(B_{1u})$	B_{1u}	3	$Q,\ T$	-	-	$\sqrt{15}xyz$
17	$\mathbb{G}_4(B_{1u})$	B_{1u}	4	$G,\ M$	-	-	$\frac{\sqrt{5}(x-y)(x+y)\left(x^2+y^2-6z^2\right)}{4}$
18	$\mathbb{Q}_2(B_{2g})$	B_{2g}	2	$Q,\ T$	-	-	$\sqrt{3}xy$
19	$\mathbb{G}_3(B_{2g})$	B_{2g}	3	$G,\ M$	-	-	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
20	$\mathbb{Q}_4(B_{2g})$	B_{2g}	4	$Q,\ T$	-	-	$-\frac{\sqrt{5}xy\left(x^2+y^2-6z^2\right)}{2}$
21	$\mathbb{G}_2(B_{2u})$	B_{2u}	2	$G,\ M$	-	-	$\sqrt{3}xy$
22	$\mathbb{Q}_3(B_{2u})$	B_{2u}	3	$Q,\ T$	-	-	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
23	$\mathbb{G}_4(B_{2u})$	B_{2u}	4	$G,\ M$	-	-	$-\frac{\sqrt{5}xy\left(x^2+y^2-6z^2\right)}{2}$
24	$\mathbb{G}_{1,1}(E_g)$	E_g	1	$G,\ M$	-	1	x
25	$\mathbb{G}_{1,2}(E_g)$					2	$-y$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
26	$\mathbb{Q}_{2,1}(E_g)$	E_g	2	$Q,\ T$	-	1	$\sqrt{3}yz$
27	$\mathbb{Q}_{2,2}(E_g)$					2	$\sqrt{3}xz$
28	$\mathbb{G}_{3,1}(E_g,1)$	E_g	3	$G,\ M$	1	1	$\frac{x\left(2x^{2}-3y^{2}-3z^{2}\right)}{2}$
29	$\mathbb{G}_{3,2}(E_g,1)$					2	$\frac{y\left(3x^{2}-2y^{2}+3z^{2}\right)}{2}$
30	$\mathbb{G}_{3,1}(E_g,2)$	E_g	3	$G,\ M$	2	1	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
31	$\mathbb{G}_{3,2}(E_g,2)$					2	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
32	$\mathbb{Q}_{4,1}(E_g,1)$	E_g	4	$Q,\ T$	1	1	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$
33	$\mathbb{Q}_{4,2}(E_g,1)$					2	$\frac{\sqrt{35}xz(x-z)(x+z)}{2}$
34	$\mathbb{Q}_{1,1}(E_u)$	E_u	1	$Q,\ T$	-	1	x
35	$\mathbb{Q}_{1,2}(E_u)$					2	y
36	$\mathbb{G}_{2,1}(E_u)$	E_u	2	$G,\ M$	-	1	$\sqrt{3}yz$
37	$\mathbb{G}_{2,2}(E_u)$					2	$-\sqrt{3}xz$
38	$\mathbb{Q}_{3,1}(E_u,1)$	E_u	3	$Q,\ T$	1	1	$\frac{x\left(2x^{2}-3y^{2}-3z^{2}\right)}{2}$
39	$\mathbb{Q}_{3,2}(E_u,1)$					2	$-\frac{y\left(3x^{2}-2y^{2}+3z^{2}\right)}{2}$
40	$\mathbb{Q}_{3,1}(E_u,2)$	E_u	3	$Q,\ T$	2	1	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
41	$\mathbb{Q}_{3,2}(E_u,2)$					2	$\frac{\sqrt{15}y(x-z)(x+z)}{2}$
42	$\mathbb{G}_{4,1}(E_u,1)$	E_u	4	$G,\ M$	1	1	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$
43	$\mathbb{G}_{4,2}(E_u,1)$					2	$-\frac{\sqrt{35}xz(x-z)(x+z)}{2}$

Basis in full matrix

Table 3: dimension = 6

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

Table 4: Atomic basis (orbital part only)

orbital	definition
$\lvert s\rangle$	1
$\lvert p_x\rangle$	x
$\lvert p_y\rangle$	y
$\lvert p_z\rangle$	z

SAMB

267 (all 267) SAMBs

- 'A' site-cluster : `A`
  * bra: $\langle s,\uparrow\rvert$, $\langle s,\downarrow\rvert$
  * ket: $\lvert s,\uparrow\rangle$, $\lvert s,\downarrow\rangle$
  * wyckoff: `2a`

$\boxed{\text{z1}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$

- 'A' site-cluster : `A`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$
  * wyckoff: `2a`

$\boxed{\text{z113}}$ $\mathbb{G}_2^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z136}}$ $\mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z153}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z171}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z192}}$ $\mathbb{Q}_{1,1}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$

$\boxed{\text{z193}}$ $\mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$

$\boxed{\text{z194}}$ $\mathbb{Q}_{1,1}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$

$\boxed{\text{z195}}$ $\mathbb{Q}_{1,2}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$

- 'A' site-cluster : `A`
  * 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: `2a`

$\boxed{\text{z2}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z3}}$ $\mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z33}}$ $\mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z48}}$ $\mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(s)}(A_{1g})$

$\boxed{\text{z63}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$

$\boxed{\text{z64}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{0}^{(s)}(A_{1g})}{2}$

- 'A'-'A' bond-cluster : `A;A_001_1`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: `4b@4c`

$\boxed{\text{z4}}$ $\mathbb{Q}_{0}^{(c)}(A_{1g}) = \mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{0}^{(b)}(A_{1g})$

$\boxed{\text{z34}}$ $\mathbb{G}_{0}^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z114}}$ $\mathbb{Q}_{1}^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z137}}$ $\mathbb{Q}_{2}^{(c)}(B_{1g}) = \mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{2}^{(b)}(B_{1g})$

$\boxed{\text{z154}}$ $\mathbb{G}_{2}^{(1,-1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z172}}$ $\mathbb{G}_{2}^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z196}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z197}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

- 'A'-'A' bond-cluster : `A;A_001_1`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$
  * wyckoff: `4b@4c`

$\boxed{\text{z5}}$ $\mathbb{Q}_{0}^{(c)}(A_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z6}}$ $\mathbb{Q}_{2}^{(1,-1;c)}(A_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z23}}$ $\mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z24}}$ $\mathbb{G}_2^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z35}}$ $\mathbb{G}_1^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z36}}$ $\mathbb{G}_1^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z49}}$ $\mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = -\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z50}}$ $\mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z65}}$ $\mathbb{Q}_2^{(c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z66}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z67}}$ $\mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z68}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z69}}$ $\mathbb{Q}_2^{(c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z70}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z71}}$ $\mathbb{Q}_3^{(1,0;c)}(B_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z72}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z115}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$

$\boxed{\text{z116}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = -\frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$

$\boxed{\text{z138}}$ $\mathbb{Q}_{2,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_{1}^{(1,0;a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z139}}$ $\mathbb{Q}_{2,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_{1}^{(1,0;a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z155}}$ $\mathbb{G}_{1,1}^{(1,-1;c)}(E_g) = -\frac{\sqrt{5}\mathbb{M}_{2}^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{M}_{2}^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{M}_{2}^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$

$\boxed{\text{z156}}$ $\mathbb{G}_{1,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{5}\mathbb{M}_{2}^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{M}_{2}^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{15}\mathbb{M}_{2}^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$

$\boxed{\text{z173}}$ $\mathbb{G}_{3,1}^{(1,-1;c)}(E_g,1) = \frac{\mathbb{M}_{2}^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\mathbb{M}_{2}^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z174}}$ $\mathbb{G}_{3,2}^{(1,-1;c)}(E_g,1) = \frac{\mathbb{M}_{2}^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\mathbb{M}_{2}^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z198}}$ $\mathbb{Q}_{1,1}^{(c)}(E_u,a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z199}}$ $\mathbb{Q}_{1,2}^{(c)}(E_u,a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z200}}$ $\mathbb{Q}_{1,1}^{(c)}(E_u,b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}$

$\boxed{\text{z201}}$ $\mathbb{Q}_{1,2}^{(c)}(E_u,b) = -\frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}$

$\boxed{\text{z202}}$ $\mathbb{Q}_{1,1}^{(1,0;c)}(E_u,a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z203}}$ $\mathbb{Q}_{1,2}^{(1,0;c)}(E_u,a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z204}}$ $\mathbb{Q}_{1,1}^{(1,0;c)}(E_u,b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}$

$\boxed{\text{z205}}$ $\mathbb{Q}_{1,2}^{(1,0;c)}(E_u,b) = -\frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}$

- 'A'-'A' bond-cluster : `A;A_001_1`
  * 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: `4b@4c`

$\boxed{\text{z7}}$ $\mathbb{Q}_0^{(c)}(A_{1g},a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z8}}$ $\mathbb{Q}_0^{(c)}(A_{1g},b) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$

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

$$\boxed{\text{z25}}\quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z37}}\quad \mathbb{G}_2^{(1,-1;c)}(A_{1u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z38}}\quad \mathbb{G}_4^{(1,-1;c)}(A_{1u},1) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$$

$\boxed{\text{z39}}$ $\mathbb{Q}_4^{(c)}(A_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{1g})$

$$\boxed{\text{z51}}\quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z73}}\quad \mathbb{Q}_3^{(1,-1;c)}(A_{2u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$$

$$\boxed{\text{z74}}\quad \mathbb{G}_4^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$$

$\boxed{\text{z75}}$ $\mathbb{Q}_2^{(c)}(B_{1g},a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z76}}$ $\mathbb{Q}_2^{(c)}(B_{1g},b) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z117}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = -\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$

$$\boxed{\text{z118}}\quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z119}}$ $\mathbb{G}_{2}^{(1,-1;c)}(B_{1u},a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z140}}$ $\mathbb{G}_{2}^{(1,-1;c)}(B_{1u},b) = \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z141}}$ $\mathbb{Q}_{2}^{(c)}(B_{2g}) = \mathbb{Q}_{2}^{(a)}(B_{2g})\mathbb{Q}_{0}^{(b)}(A_{1g})$

$\boxed{\text{z142}}$ $\mathbb{Q}_{3}^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{30}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} - \frac{\sqrt{30}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$

$\boxed{\text{z157}}$ $\mathbb{G}_{2}^{(1,-1;c)}(B_{2u},a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z158}}$ $\mathbb{G}_{2}^{(1,-1;c)}(B_{2u},b) = -\frac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{30}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \frac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \frac{\sqrt{30}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$

$\boxed{\text{z159}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g,a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z175}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g,a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z176}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g,b) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}$

$\boxed{\text{z177}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g,b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{1g})}{2}$

$\boxed{\text{z206}}$ $\mathbb{Q}_{1,1}^{(c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1}^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z207}}$ $\mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_{1}^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z208}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z209}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

z210 $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,1) = -\frac{\sqrt{2}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

z211 $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,1) = -\frac{\sqrt{2}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

z212 $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,2) = \frac{\sqrt{2}\mathbb{M}_{3}^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

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

- 'A'-'A' bond-cluster : `A;A_002_1`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  * wyckoff: `8a@8f`

z10 $\mathbb{Q}_{0}^{(c)}(A_{1g}) = \mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{0}^{(b)}(A_{1g})$

z52 $\mathbb{G}_{0}^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$

z77 $\mathbb{G}_{2}^{(1,-1;c)}(A_{1u}) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$

z78 $\mathbb{Q}_{1}^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

z120 $\mathbb{G}_{2}^{(1,-1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

z121 $\mathbb{Q}_{2}^{(c)}(B_{2g}) = \mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{2}^{(b)}(B_{2g})$

z143 $\mathbb{Q}_{3}^{(1,-1;c)}(B_{2u}) = \mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{M}_{2}^{(b)}(B_{1u})$

z160 $\mathbb{G}_{2}^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

z178 $\mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z179}}$ $\mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z214}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u,a) = -\frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z215}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u,a) = -\frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z216}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u,b) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{1u})}{2}$

$\boxed{\text{z217}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u,b) = \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{1u})}{2}$

$\boxed{\text{z218}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E_u) = -\frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z219}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E_u) = -\frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

- 'A'-'A' bond-cluster : `A;A_002_1`
  * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  * ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$
  * wyckoff: `8a@8f`

$\boxed{\text{z11}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z12}}$ $\mathbb{Q}_0^{(1,-1;c)}(A_{1g}) = \mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{M}_2^{(b)}(B_{1u})$

$\boxed{\text{z13}}$ $\mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z14}}$ $\mathbb{Q}_0^{(1,0;c)}(A_{1g}) = \mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z26}}$ $\mathbb{G}_2^{(c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z27}}$ $\mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_2^{(b)}(B_{2g})$

$\boxed{\text{z28}}$ $\mathbb{G}_2^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z29}}$ $\mathbb{G}_2^{(1,0;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z40}}$ $\mathbb{Q}_4^{(1,-1;c)}(A_{2g}) = \mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{M}_2^{(b)}(B_{1u})$

$\boxed{\text{z41}}$ $\mathbb{G}_1^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z42}}$ $\mathbb{G}_1^{(1,-1;c)}(A_{2g}) = \frac{\sqrt{30}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{30}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_1^{(b)}(A_{2u})}{5}$

$\boxed{\text{z43}}$ $\mathbb{G}_3^{(1,-1;c)}(A_{2g}) = -\frac{\sqrt{5}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{5} + \frac{\sqrt{5}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{5} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_1^{(b)}(A_{2u})}{5}$

$\boxed{\text{z53}}$ $\mathbb{Q}_1^{(c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z54}}$ $\mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_2^{(b)}(B_{2g})$

$\boxed{\text{z55}}$ $\mathbb{Q}_1^{(1,0;c)}(A_{2u}, a) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z56}}$ $\mathbb{Q}_1^{(1,0;c)}(A_{2u}, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z79}}$ $\mathbb{Q}_2^{(c)}(B_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z80}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}, a) = -\frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$

$\boxed{\text{z81}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}, b) = -\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{M}_2^{(b)}(B_{1u})$

$\boxed{\text{z82}}$ $\mathbb{G}_3^{(1,-1;c)}(B_{1g}) = \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$

$\boxed{\text{z83}}$ $\mathbb{Q}_3^{(c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z84}}$ $$\mathbb{Q}_3^{(1,0;c)}(B_{1u}) = \frac{\sqrt{3}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} + \frac{\sqrt{3}\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{2g})}{3}$$

$\boxed{\text{z85}}$ $$\mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$\boxed{\text{z86}}$ $$\mathbb{G}_2^{(1,0;c)}(B_{1u}) = \frac{\sqrt{6}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\sqrt{6}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} - \frac{\sqrt{6}\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_2^{(b)}(B_{2g})}{3}$$

$\boxed{\text{z87}}$ $$\mathbb{Q}_2^{(c)}(B_{2g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$\boxed{\text{z88}}$ $$\mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} - \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$\boxed{\text{z89}}$ $$\mathbb{Q}_2^{(1,0;c)}(B_{2g}) = \mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{M}_2^{(b)}(B_{1u})$$

$\boxed{\text{z90}}$ $$\mathbb{G}_3^{(1,-1;c)}(B_{2g}) = -\frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$\boxed{\text{z91}}$ $$\mathbb{Q}_3^{(c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$\boxed{\text{z92}}$ $$\mathbb{Q}_3^{(1,-1;c)}(B_{2u}) = -\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_2^{(b)}(B_{2g})$$

$\boxed{\text{z93}}$ $$\mathbb{Q}_3^{(1,0;c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$\boxed{\text{z94}}$ $$\mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$$

$\boxed{\text{z122}}$ $$\mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$\boxed{\text{z123}}$ $$\mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$\boxed{\text{z124}}$ $$\mathbb{Q}_{2,1}^{(c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{M}_2^{(b)}(B_{1u})}{2}$$

$\boxed{\text{z125}}$ $$\mathbb{Q}_{2,2}^{(c)}(E_g, b) = -\frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{M}_2^{(b)}(B_{1u})}{2}$$

$\boxed{\text{z144}}$ $$\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g,a) = \frac{\sqrt{3}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{6} + \frac{\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{6}$$

$\boxed{\text{z145}}$ $$\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g,a) = \frac{\sqrt{3}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{6} - \frac{\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{6} - \frac{\sqrt{3}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{6}$$

$\boxed{\text{z146}}$ $$\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g,b) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{M}_2^{(b)}(B_{1u})}{2}$$

$\boxed{\text{z147}}$ $$\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g,b) = -\frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{M}_2^{(b)}(B_{1u})}{2}$$

$\boxed{\text{z161}}$ $$\mathbb{Q}_{2,1}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$\boxed{\text{z162}}$ $$\mathbb{Q}_{2,2}^{(1,0;c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$\boxed{\text{z163}}$ $$\mathbb{G}_{1,1}^{(1,-1;c)}(E_g) = -\frac{\sqrt{15}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$$

$\boxed{\text{z164}}$ $$\mathbb{G}_{1,2}^{(1,-1;c)}(E_g) = -\frac{\sqrt{15}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} + \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \frac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$$

$\boxed{\text{z180}}$ $$\mathbb{G}_{3,1}^{(1,-1;c)}(E_g,1) = \frac{\sqrt{10}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{10} - \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{20} - \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$$

$\boxed{\text{z181}}$ $$\mathbb{G}_{3,2}^{(1,-1;c)}(E_g,1) = \frac{\sqrt{10}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{10} + \frac{\sqrt{30}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{20} + \frac{3\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{20} + \frac{\sqrt{10}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$$

$\boxed{\text{z182}}$ $$\mathbb{G}_{3,1}^{(1,-1;c)}(E_g,2) = \frac{\sqrt{6}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{6} - \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{6}$$

$\boxed{\text{z183}}$ $$\mathbb{G}_{3,2}^{(1,-1;c)}(E_g,2) = \frac{\sqrt{6}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{6} + \frac{\sqrt{2}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{12} - \frac{\sqrt{6}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{6}$$

$\boxed{\text{z220}}$ $$\mathbb{Q}_{1,1}^{(c)}(E_u,a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z221}}$ $$\mathbb{Q}_{1,2}^{(c)}(E_u,a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z222}}$ $$\mathbb{Q}_{1,1}^{(c)}(E_u, b) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{2g})}{2}$$

$\boxed{\text{z223}}$ $$\mathbb{Q}_{1,2}^{(c)}(E_u, b) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{2g})}{2}$$

$\boxed{\text{z224}}$ $$\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{30}\mathbb{G}_{2}^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{10}\mathbb{G}_{2}^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{10}\mathbb{G}_{2}^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}$$

$\boxed{\text{z225}}$ $$\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{30}\mathbb{G}_{2}^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{10}\mathbb{G}_{2}^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{10}\mathbb{G}_{2}^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}$$

$\boxed{\text{z226}}$ $$\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 1) = \frac{\sqrt{30}\mathbb{G}_{2}^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} + \frac{\sqrt{10}\mathbb{G}_{2}^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} + \frac{\sqrt{10}\mathbb{G}_{2}^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{5}$$

$\boxed{\text{z227}}$ $$\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 1) = -\frac{\sqrt{30}\mathbb{G}_{2}^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{20} + \frac{\sqrt{10}\mathbb{G}_{2}^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{20} - \frac{\sqrt{10}\mathbb{G}_{2}^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5}$$

$\boxed{\text{z228}}$ $$\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 2) = \frac{\sqrt{2}\mathbb{G}_{2}^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{G}_{2}^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4}$$

$\boxed{\text{z229}}$ $$\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 2) = -\frac{\sqrt{2}\mathbb{G}_{2}^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{G}_{2}^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4}$$

$\boxed{\text{z230}}$ $$\mathbb{Q}_{1,1}^{(1,0;c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z231}}$ $$\mathbb{Q}_{1,2}^{(1,0;c)}(E_u, a) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z232}}$ $$\mathbb{Q}_{1,1}^{(1,0;c)}(E_u, b) = \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{2g})}{2} + \frac{\mathbb{Q}_{1}^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$\boxed{\text{z233}}$ $$\mathbb{Q}_{1,2}^{(1,0;c)}(E_u, b) = \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{2g})}{2} + \frac{\mathbb{Q}_{1}^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$\boxed{\text{z234}}$ $$\mathbb{Q}_{3,1}^{(1,0;c)}(E_u, 2) = \frac{\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{2g})}{2} - \frac{\mathbb{Q}_{1}^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$\boxed{\text{z235}}$ $$\mathbb{Q}_{3,2}^{(1,0;c)}(E_u, 2) = \frac{\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_{2}^{(b)}(B_{2g})}{2} - \frac{\mathbb{Q}_{1}^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

- 'A'-'A' bond-cluster : `A;A_002_1`
  - * 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: `8a@8f`

$\boxed{\text{z15}}$ $\mathbb{Q}_0^{(c)}(A_{1g},a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z16}}$ $\mathbb{Q}_0^{(c)}(A_{1g},b) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_2^{(b)}(B_{2g})$

$\boxed{\text{z17}}$ $\mathbb{Q}_0^{(1,-1;c)}(A_{1g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z18}}$ $\mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z30}}$ $\mathbb{Q}_5^{(1,-1;c)}(A_{1u}) = \mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{M}_2^{(b)}(B_{1u})$

$\boxed{\text{z31}}$ $\mathbb{G}_0^{(c)}(A_{1u}) = \mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z44}}$ $\mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \frac{\sqrt{3}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$

$\boxed{\text{z45}}$ $\mathbb{G}_2^{(1,-1;c)}(A_{1u},a) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \frac{\sqrt{6}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$

$\boxed{\text{z57}}$ $\mathbb{G}_2^{(1,-1;c)}(A_{1u},b) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$

$\boxed{\text{z58}}$ $\mathbb{G}_4^{(1,-1;c)}(A_{1u},1) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$

$\boxed{\text{z59}}$ $\mathbb{Q}_4^{(c)}(A_{2g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$

$\boxed{\text{z60}}$ $\mathbb{G}_1^{(1,-1;c)}(A_{2g}) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z95}}$ $\mathbb{Q}_1^{(1,-1;c)}(A_{2u},a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z96}}$ $\mathbb{Q}_1^{(1,-1;c)}(A_{2u},b) = \mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{M}_2^{(b)}(B_{1u})$

$\boxed{\text{z97}}$ $\mathbb{Q}_3^{(1,-1;c)}(A_{2u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$

$\boxed{\text{z98}}$ $\mathbb{G}_4^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$

$\boxed{\text{z99}}$ $\mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z100}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z101}}$ $\mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$

$\boxed{\text{z102}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u},a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z103}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u},b) = \frac{3\sqrt{7}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{105}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{42} + \frac{3\sqrt{7}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{14}$
$- \frac{\sqrt{105}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{42} + \frac{\sqrt{105}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g})\mathbb{T}_{1}^{(b)}(A_{2u})}{21}$

$\boxed{\text{z104}}$ $\mathbb{G}_4^{(1,-1;c)}(B_{1u}) = \frac{\sqrt{35}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{35}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g})\mathbb{T}_{1}^{(b)}(A_{2u})}{7}$

$\boxed{\text{z105}}$ $\mathbb{Q}_2^{(c)}(B_{2g},a) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$

$\boxed{\text{z106}}$ $\mathbb{Q}_2^{(c)}(B_{2g},b) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z126}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{10}\mathbb{Q}_{2}^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2}^{(b)}(B_{2g})}{5}$

$\boxed{\text{z127}}$ $\mathbb{Q}_4^{(1,-1;c)}(B_{2g}) = \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} + \frac{\sqrt{15}\mathbb{Q}_{2}^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2}^{(b)}(B_{2g})}{5}$

$\boxed{\text{z128}}$ $\mathbb{Q}_3^{(c)}(B_{2u}) = \mathbb{M}_1^{(a)}(A_{2g})\mathbb{M}_2^{(b)}(B_{1u})$

$\boxed{\text{z129}}$ $\mathbb{Q}_3^{(1,-1;c)}(B_{2u},a) = \mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{M}_2^{(b)}(B_{1u})$

$\boxed{\text{z130}}$ $$\mathbb{Q}_{3}^{(1,-1;c)}(B_{2u},b) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{12} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{3}\mathbb{M}_{3}^{(1,-1;a)}(B_{1g})\mathbb{T}_{1}^{(b)}(A_{2u})}{3}$$

$\boxed{\text{z131}}$ $$\mathbb{G}_{2}^{(1,-1;c)}(B_{2u},a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$\boxed{\text{z148}}$ $$\mathbb{G}_{2}^{(1,-1;c)}(B_{2u},b) = -\frac{\sqrt{7}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{7} + \frac{\sqrt{105}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{21} + \frac{\sqrt{7}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{7} - \frac{\sqrt{105}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{21} + \frac{\sqrt{105}\mathbb{M}_{3}^{(1,-1;a)}(B_{1g})\mathbb{T}_{1}^{(b)}(A_{2u})}{21}$$

$\boxed{\text{z149}}$ $$\mathbb{G}_{4}^{(1,-1;c)}(B_{2u}) = -\frac{\sqrt{35}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{28} - \frac{3\sqrt{21}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{28} + \frac{\sqrt{35}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{28} + \frac{3\sqrt{21}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{28} + \frac{\sqrt{21}\mathbb{M}_{3}^{(1,-1;a)}(B_{1g})\mathbb{T}_{1}^{(b)}(A_{2u})}{7}$$

$\boxed{\text{z150}}$ $$\mathbb{Q}_{2,1}^{(c)}(E_g,a) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$\boxed{\text{z151}}$ $$\mathbb{Q}_{2,2}^{(c)}(E_g,a) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$\boxed{\text{z165}}$ $$\mathbb{Q}_{2,1}^{(c)}(E_g,b) = -\frac{\mathbb{Q}_{2}^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\mathbb{Q}_{2}^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$\boxed{\text{z166}}$ $$\mathbb{Q}_{2,2}^{(c)}(E_g,b) = \frac{\mathbb{Q}_{2}^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\mathbb{Q}_{2}^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$\boxed{\text{z167}}$ $$\mathbb{Q}_{4,1}^{(c)}(E_g,1) = -\frac{\mathbb{Q}_{2}^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\mathbb{Q}_{2}^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$\boxed{\text{z168}}$ $$\mathbb{Q}_{4,2}^{(c)}(E_g,1) = \frac{\mathbb{Q}_{2}^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\mathbb{Q}_{2}^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$\boxed{\text{z184}}$ $$\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g,a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z185}}$ $$\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g,a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z186}}$ $$\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g,b) = \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{2g})}{4} + \frac{\sqrt{2}\mathbb{Q}_{2}^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4}$$

$\boxed{\text{z187}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g,b)=\frac{\sqrt{6}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{2g})}{4}+\frac{\sqrt{2}\mathbb{Q}_{2}^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4}$

$\boxed{\text{z188}}$ $\mathbb{Q}_{4,1}^{(1,-1;c)}(E_g,1)=\frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{2g})}{4}-\frac{\sqrt{6}\mathbb{Q}_{2}^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4}$

$\boxed{\text{z189}}$ $\mathbb{Q}_{4,2}^{(1,-1;c)}(E_g,1)=\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2}^{(b)}(B_{2g})}{4}-\frac{\sqrt{6}\mathbb{Q}_{2}^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4}$

$\boxed{\text{z236}}$ $\mathbb{Q}_{1,1}^{(c)}(E_u)=-\frac{\sqrt{2}\mathbb{M}_{1}^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z237}}$ $\mathbb{Q}_{1,2}^{(c)}(E_u)=\frac{\sqrt{2}\mathbb{M}_{1}^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z238}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u,a)=-\frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1}^{(b)}(A_{2u})}{2}-\frac{\mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z239}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u,a)=-\frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1}^{(b)}(A_{2u})}{2}+\frac{\mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z240}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u,b)=\frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{M}_{2}^{(b)}(B_{1u})}{2}$

$\boxed{\text{z241}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u,b)=\frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{M}_{2}^{(b)}(B_{1u})}{2}$

$\boxed{\text{z242}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u,c)=\frac{3\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{M}_{2}^{(b)}(B_{1u})}{8}-\frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{M}_{2}^{(b)}(B_{1u})}{8}$

$\boxed{\text{z243}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u,c)=\frac{3\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{M}_{2}^{(b)}(B_{1u})}{8}-\frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{M}_{2}^{(b)}(B_{1u})}{8}$

$\boxed{\text{z244}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,1a)=\frac{\sqrt{78}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1}^{(b)}(A_{2u})}{26}-\frac{\sqrt{130}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1}^{(b)}(A_{2u})}{26}-\frac{\sqrt{130}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{26}$

$\boxed{\text{z245}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,1a)=\frac{\sqrt{78}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1}^{(b)}(A_{2u})}{26}-\frac{\sqrt{130}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1}^{(b)}(A_{2u})}{26}-\frac{\sqrt{130}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{26}$

$\boxed{\text{z246}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,1b)=\frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{M}_{2}^{(b)}(B_{1u})}{8}+\frac{3\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{M}_{2}^{(b)}(B_{1u})}{8}$

$\boxed{\text{z247}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,1b) = \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{M}_{2}^{(b)}(B_{1u})}{8} + \frac{3\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{M}_{2}^{(b)}(B_{1u})}{8}$

$\boxed{\text{z248}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,2) = -\frac{5\sqrt{65}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1}^{(b)}(A_{2u})}{104} - \frac{\sqrt{39}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1}^{(b)}(A_{2u})}{312} + \frac{\sqrt{39}\mathbb{M}_{3}^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{12} - \frac{7\sqrt{39}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{156}$

$\boxed{\text{z249}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,2) = -\frac{5\sqrt{65}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1}^{(b)}(A_{2u})}{104} - \frac{\sqrt{39}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1}^{(b)}(A_{2u})}{312} - \frac{\sqrt{39}\mathbb{M}_{3}^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{12} - \frac{7\sqrt{39}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{156}$

$\boxed{\text{z250}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E_u,a) = -\frac{\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1}^{(b)}(A_{2u})}{2} + \frac{\mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z251}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E_u,a) = -\frac{\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1}^{(b)}(A_{2u})}{2} - \frac{\mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z252}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E_u,b) = \frac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1}^{(b)}(A_{2u})}{8} + \frac{5\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1}^{(b)}(A_{2u})}{24} + \frac{\sqrt{6}\mathbb{M}_{3}^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{12} - \frac{\sqrt{6}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{12}$

$\boxed{\text{z253}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E_u,b) = \frac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1}^{(b)}(A_{2u})}{8} + \frac{5\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1}^{(b)}(A_{2u})}{24} - \frac{\sqrt{6}\mathbb{M}_{3}^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{12} - \frac{\sqrt{6}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{12}$

$\boxed{\text{z254}}$ $\mathbb{G}_{4,1}^{(1,-1;c)}(E_u,1) = -\frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1}^{(b)}(A_{2u})}{8} + \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1}^{(b)}(A_{2u})}{8} - \frac{\sqrt{3}\mathbb{M}_{3}^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$

$\boxed{\text{z255}}$ $\mathbb{G}_{4,2}^{(1,-1;c)}(E_u,1) = -\frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1}^{(b)}(A_{2u})}{8} + \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1}^{(b)}(A_{2u})}{8} + \frac{\sqrt{3}\mathbb{M}_{3}^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3}^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$

- 'A'-'A' bond-cluster : `A;A_007_1`
  - * bra: $\langle s,\uparrow|$, $\langle s,\downarrow|$
  - * ket: $|s,\uparrow\rangle$, $|s,\downarrow\rangle$
  - * wyckoff: `2a@2b`

$\boxed{\text{z19}}$ $\mathbb{Q}_{0}^{(c)}(A_{1g}) = \mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{0}^{(b)}(A_{1g})$

$\boxed{\text{z132}}$ $\mathbb{G}_{0}^{(1,-1;c)}(A_{1u}) = \mathbb{M}_{1}^{(1,-1;a)}(A_{2g})\mathbb{T}_{1}^{(b)}(A_{2u})$

$\boxed{\text{z256}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1}^{(b)}(A_{2u})}{2}$

$\boxed{\text{z257}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

- 'A'-'A' bond-cluster : `A;A_007_1`
  * bra: $\langle s, \uparrow|$, $\langle s, \downarrow|$
  * ket: $|p_x, \uparrow\rangle$, $|p_x, \downarrow\rangle$, $|p_y, \uparrow\rangle$, $|p_y, \downarrow\rangle$
  * wyckoff: `2a@2b`

$\boxed{\text{z20}}$ $\mathbb{Q}_0^{(1,0;c)}(A_{1g}) = \mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z32}}$ $\mathbb{G}_2^{(1,-1;c)}(A_{1u}) = \mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z46}}$ $\mathbb{G}_1^{(1,-1;c)}(A_{2g}) = \mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z61}}$ $\mathbb{Q}_1^{(1,0;c)}(A_{2u}) = \mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z107}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{1g}) = \mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z108}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z109}}$ $\mathbb{Q}_2^{(1,-1;c)}(B_{2g}) = -\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z110}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z133}}$ $\mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z152}}$ $\mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z169}}$ $\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z190}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z258}}$ $\mathbb{Q}_{1,1}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z259}}$ $$\mathbb{Q}_{1,2}^{(c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z260}}$ $$\mathbb{Q}_{1,1}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z261}}$ $$\mathbb{Q}_{1,2}^{(1,0;c)}(E_u) = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

- 'A'-'A' bond-cluster : `A;A_007_1`
  * 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: `2a@2b`

$\boxed{\text{z21}}$ $$\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$\boxed{\text{z22}}$ $$\mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = \mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$\boxed{\text{z47}}$ $$\mathbb{G}_0^{(c)}(A_{1u}) = \mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})$$

$\boxed{\text{z62}}$ $$\mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})$$

$\boxed{\text{z111}}$ $$\mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$\boxed{\text{z112}}$ $$\mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = -\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})$$

$\boxed{\text{z134}}$ $$\mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$\boxed{\text{z135}}$ $$\mathbb{Q}_3^{(1,-1;c)}(B_{2u}) = \mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})$$

$\boxed{\text{z170}}$ $$\mathbb{Q}_{2,1}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z191}}$ $$\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z262}}$ $$\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$$

$\boxed{\text{z263}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

$\boxed{\text{z264}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,1) = \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{4} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{4}$

$\boxed{\text{z265}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,1) = \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{4} - \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{4}$

$\boxed{\text{z266}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,2) = -\frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{4}$

$\boxed{\text{z267}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,2) = -\frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{4} - \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{4}$

Atomic SAMB

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

$\boxed{\text{x1}}$ $\mathbb{Q}_0^{(a)}(A_{1g}) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$

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

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

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

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

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

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

$\boxed{\text{x7}}$ $\mathbb{Q}_{1}^{(1,0;a)}(A_{2u}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} \\ \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$

$\boxed{\text{x8}}$ $\mathbb{Q}_{1,1}^{(1,0;a)}(E_u) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & \frac{i}{2} \end{bmatrix}$

$\boxed{\text{x9}}$ $\mathbb{Q}_{1,2}^{(1,0;a)}(E_u) = \begin{bmatrix} \frac{i}{2} & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 \end{bmatrix}$

$\boxed{\text{x10}}$ $\mathbb{G}_{2}^{(1,-1;a)}(A_{1u}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 \end{bmatrix}$

$\boxed{\text{x11}}$ $\mathbb{G}_{2}^{(1,-1;a)}(B_{1u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & -\frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 \end{bmatrix}$

$\boxed{\text{x12}}$ $\mathbb{G}_{2}^{(1,-1;a)}(B_{2u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} \\ -\frac{\sqrt{2}}{4} & 0 & \frac{\sqrt{2}i}{4} & 0 \end{bmatrix}$

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

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

$\boxed{\text{x15}}$ $\mathbb{M}_{2}^{(1,-1;a)}(B_{2u}) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} \\ \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 \end{bmatrix}$

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

$\boxed{\text{x17}}$ $\mathbb{M}_{2,2}^{(1,-1;a)}(E_u) = \begin{bmatrix} -\frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$

$\boxed{\text{x18}}$ $\mathbb{T}_{1,1}^{(a)}(E_u) = \begin{bmatrix} \frac{i}{2} & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$

$\boxed{\text{x19}}$ $\mathbb{T}_{1,2}^{(a)}(E_u) = \begin{bmatrix} 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & 0 & \frac{i}{2} \end{bmatrix}$

$\boxed{\text{x20}}$ $\mathbb{T}_{1}^{(1,0;a)}(A_{2u}) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} \\ -\frac{\sqrt{2}i}{4} & 0 & \frac{\sqrt{2}}{4} & 0 \end{bmatrix}$

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

$\boxed{\text{x21}}$ $\mathbb{Q}_{0}^{(a)}(A_{1g}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$

$\boxed{\text{x22}}$ $\mathbb{Q}_{2}^{(a)}(B_{1g}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$

$\boxed{\text{x23}}$ $\mathbb{Q}_{2}^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$

$\boxed{\text{x24}}$ $\mathbb{Q}_{2}^{(1,-1;a)}(A_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 \end{bmatrix}$

$\boxed{\text{x25}}$ $\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x26}}$ $\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g) = \begin{bmatrix} 0 & 0 & 0 & -\frac{i}{2} \\ 0 & 0 & -\frac{i}{2} & 0 \\ 0 & \frac{i}{2} & 0 & 0 \\ \frac{i}{2} & 0 & 0 & 0 \end{bmatrix}$

$\boxed{\text{x27}}$ $\mathbb{M}_{1}^{(a)}(A_{2g}) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$

$\boxed{\text{x28}}$ $\mathbb{M}_{1}^{(1,-1;a)}(A_{2g}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$

$\boxed{\text{x29}}$ $\mathbb{M}_{3}^{(1,-1;a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \end{bmatrix}$

$\boxed{\text{x30}}$ $\mathbb{M}_{3}^{(1,-1;a)}(B_{2g}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$

$\boxed{\text{x31}}$ $\mathbb{M}_{1,1}^{(1,-1;a)}(E_{g}) = \begin{bmatrix} 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \end{bmatrix}$

$\boxed{\text{x32}}$ $\mathbb{M}_{1,2}^{(1,-1;a)}(E_{g}) = \begin{bmatrix} 0 & \frac{i}{2} & 0 & 0 \\ -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ 0 & 0 & -\frac{i}{2} & 0 \end{bmatrix}$

$\boxed{\text{x33}}$ $\mathbb{M}_{3,1}^{(1,-1;a)}(E_{g},1) = \begin{bmatrix} 0 & \frac{3\sqrt{13}}{26} & 0 & \frac{\sqrt{13}i}{13} \\ \frac{3\sqrt{13}}{26} & 0 & -\frac{\sqrt{13}i}{13} & 0 \\ 0 & \frac{\sqrt{13}i}{13} & 0 & -\frac{3\sqrt{13}}{26} \\ -\frac{\sqrt{13}i}{13} & 0 & -\frac{3\sqrt{13}}{26} & 0 \end{bmatrix}$

$\boxed{\text{x34}}$ $\mathbb{M}_{3,2}^{(1,-1;a)}(E_{g},1) = \begin{bmatrix} 0 & -\frac{3\sqrt{13}i}{26} & 0 & \frac{\sqrt{13}}{13} \\ \frac{3\sqrt{13}i}{26} & 0 & \frac{\sqrt{13}}{13} & 0 \\ 0 & \frac{\sqrt{13}}{13} & 0 & \frac{3\sqrt{13}i}{26} \\ \frac{\sqrt{13}}{13} & 0 & -\frac{3\sqrt{13}i}{26} & 0 \end{bmatrix}$

$\boxed{\text{x35}}$ $\mathbb{M}_{3,1}^{(1,-1;a)}(E_{g},2) = \begin{bmatrix} 0 & \frac{\sqrt{13}}{13} & 0 & -\frac{3\sqrt{13}i}{26} \\ \frac{\sqrt{13}}{13} & 0 & \frac{3\sqrt{13}i}{26} & 0 \\ 0 & -\frac{3\sqrt{13}i}{26} & 0 & -\frac{\sqrt{13}}{13} \\ \frac{3\sqrt{13}i}{26} & 0 & -\frac{\sqrt{13}}{13} & 0 \end{bmatrix}$

$\boxed{\text{x36}}$ $\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2) = \begin{bmatrix} 0 & -\frac{\sqrt{13}i}{13} & 0 & -\frac{3\sqrt{13}}{26} \\ \frac{\sqrt{13}i}{13} & 0 & -\frac{3\sqrt{13}}{26} & 0 \\ 0 & -\frac{3\sqrt{13}}{26} & 0 & \frac{\sqrt{13}i}{13} \\ -\frac{3\sqrt{13}}{26} & 0 & -\frac{\sqrt{13}i}{13} & 0 \end{bmatrix}$

Cluster SAMB

- Site cluster

** Wyckoff: `2a`

$\boxed{\text{y1}}$ $\mathbb{Q}_0^{(s)}(A_{1g}) = [1]$

- Bond cluster

** Wyckoff: `2a@2b`

$\boxed{\text{y2}}$ $\mathbb{Q}_0^{(s)}(A_{1g}) = [1]$

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

** Wyckoff: `4b@4c`

$\boxed{\text{y4}}$ $\mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right]$

$\boxed{\text{y5}}$ $\mathbb{Q}_2^{(s)}(B_{1g}) = \left[\frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}\right]$

$\boxed{\text{y6}}$ $\mathbb{T}_{1,1}^{(s)}(E_u) = [0, -i]$

$\boxed{\text{y7}}$ $\mathbb{T}_{1,2}^{(s)}(E_u) = [i, 0]$

** Wyckoff: `8a@8f`

$\boxed{\text{y8}}$ $\mathbb{Q}_0^{(s)}(A_{1g}) = \left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$

$\boxed{\text{y9}}$ $\mathbb{T}_1^{(s)}(A_{2u}) = \left[\frac{i}{2}, \frac{i}{2}, \frac{i}{2}, \frac{i}{2}\right]$

$\boxed{\text{y10}}$ $\mathbb{M}_2^{(s)}(B_{1u}) = \left[\frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, -\frac{i}{2}\right]$

$\boxed{\text{y11}}$ $\mathbb{Q}_2^{(s)}(B_{2g}) = \left[\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\right]$

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

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

$\boxed{\text{y14}}$ $\mathbb{T}_{1,1}^{(s)}(E_u) = \left[\frac{i}{2}, -\frac{i}{2}, -\frac{i}{2}, \frac{i}{2}\right]$

$\boxed{\text{y15}}$ $\mathbb{T}_{1,2}^{(s)}(E_u) = \left[\frac{i}{2}, -\frac{i}{2}, \frac{i}{2}, -\frac{i}{2}\right]$

Site and Bond

Table 5: Orbital of each site

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

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	`A`	`A`	`[1,2,7]`	`[s,p]`	`[s,p]`

Site in Unit Cell

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

Table 7: 'A' (#1) site cluster (2a), 4/mmm

SL	position ($\boldsymbol{s}$)	mapping
1	`[ 0.00000, 0.00000, 0.00000]`	`[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16]`

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 (4b@4c), ND, $|\boldsymbol{v}|$= 1.0 (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,-2,5,-6,-9,10,-13,14]	(1,1)	(1,1)	[-1,0,-1]
2	[-1.00000, 0.00000, 0.00000]	[0.50000, 0.00000, 0.00000]	[3,-4,-7,8,-11,12,15,-16]	(1,1)	(1,1)	[0,1,1]

Table 9: 2-th 'A'-'A' [1] (#2) bond cluster (8a@8f), ND, $|\boldsymbol{v}|$= 1.35853 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[-0.50000,-0.50000,-0.50000]	[0.25000, 0.25000, 0.25000]	[1,-8,-9,16]	(1,1)	(1,2)	[1,1,1]
2	[0.50000, 0.50000,-0.50000]	[0.75000, 0.75000, 0.25000]	[2,-7,-10,15]	(1,1)	(1,2)	[0,0,-1]
3	[0.50000,-0.50000,-0.50000]	[0.75000, 0.25000, 0.25000]	[3,-6,-11,14]	(1,1)	(1,2)	[1,0,0]
4	[-0.50000, 0.50000,-0.50000]	[0.25000, 0.75000, 0.25000]	[4,-5,-12,13]	(1,1)	(1,2)	[0,1,0]