Model for "BCT"

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 …

2

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	$-y$

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	$\frac{x(2x^2-3y^2-3z^2)}{2}$
29	$\mathbb{G}_{3,2}(E_g,1)$					2	$\frac{y(3x^2-2y^2+3z^2)}{2}$
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	$\frac{x(2x^2-3y^2-3z^2)}{2}$
39	$\mathbb{Q}_{3,2}(E_u,1)$					2	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
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	$|s,\uparrow\rangle$ @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)								

Table 4: Atomic basis (orbital part only)

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

━━ **SAMB** ━━

204 (all 267) SAMBs

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{z64}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

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

$$\boxed{\text{z4}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$$

$$\boxed{\text{z34}} \quad \mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z114}} \quad \mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z137}} \quad \mathbb{Q}_2^{(c)}(B_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$$

$$\boxed{\text{z154}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z172}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z196}} \quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z197}} \quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

- 'A'-'A' bond-cluster
  * 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`

$$\boxed{\text{z5}} \quad \mathbb{Q}_0^{(c)}(A_{1g}) = \frac{\sqrt{2}\mathbb{T}_{1,1}^{(a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \frac{\sqrt{2}\mathbb{T}_{1,2}^{(a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z6}} \quad \mathbb{Q}_2^{(1,-1;c)}(A_{1g}) = -\frac{\sqrt{2}\mathbb{M}_{2,1}^{(1,-1;a)}(E_u)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{2,2}^{(1,-1;a)}(E_u)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$$

7

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$\boxed{\text{z138}}$ $\quad \mathbb{Q}_{2,1}^{(1,0;c)}(E_g) = \dfrac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z139}}$ $\quad \mathbb{Q}_{2,2}^{(1,0;c)}(E_g) = \dfrac{\sqrt{2}\mathbb{T}_1^{(1,0;a)}(A_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z155}}$ $\quad \mathbb{G}_{1,1}^{(1,-1;c)}(E_g) = -\dfrac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{5} + \dfrac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10} + \dfrac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10}$

$\boxed{\text{z156}}$ $\quad \mathbb{G}_{1,2}^{(1,-1;c)}(E_g) = \dfrac{\sqrt{5}\mathbb{M}_2^{(1,-1;a)}(A_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{5} + \dfrac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{10} - \dfrac{\sqrt{15}\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{10}$

$\boxed{\text{z173}}$ $\quad \mathbb{G}_{3,1}^{(1,-1;c)}(E_g,1) = \dfrac{\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2} - \dfrac{\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z174}}$ $\quad \mathbb{G}_{3,2}^{(1,-1;c)}(E_g,1) = \dfrac{\mathbb{M}_2^{(1,-1;a)}(B_{1u})\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \dfrac{\mathbb{M}_2^{(1,-1;a)}(B_{2u})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z198}}$ $\quad \mathbb{Q}_{1,1}^{(c)}(E_u,a) = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z199}}$ $\quad \mathbb{Q}_{1,2}^{(c)}(E_u,a) = \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z200}}$ $\quad \mathbb{Q}_{1,1}^{(c)}(E_u,b) = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$

$\boxed{\text{z201}}$ $\quad \mathbb{Q}_{1,2}^{(c)}(E_u,b) = -\dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$

$\boxed{\text{z202}}$ $\quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u,a) = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z203}}$ $\quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u,a) = \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z204}}$ $\quad \mathbb{Q}_{1,1}^{(1,0;c)}(E_u,b) = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$

$\boxed{\text{z205}}$ $\quad \mathbb{Q}_{1,2}^{(1,0;c)}(E_u,b) = -\dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

10

$\boxed{\text{z119}}$ $\quad \mathbb{G}_2^{(1,-1;c)}(B_{1u},a) = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z140}}$ $\quad \mathbb{G}_2^{(1,-1;c)}(B_{1u},b) = \dfrac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \dfrac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z141}}$ $\quad \mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z142}}$ $\quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u}) = \dfrac{\sqrt{30}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \dfrac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} - \dfrac{\sqrt{30}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \dfrac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$

$\boxed{\text{z157}}$ $\quad \mathbb{G}_2^{(1,-1;c)}(B_{2u},a) = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z158}}$ $\quad \mathbb{G}_2^{(1,-1;c)}(B_{2u},b) = -\dfrac{\sqrt{2}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \dfrac{\sqrt{30}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{8} + \dfrac{\sqrt{2}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{8} - \dfrac{\sqrt{30}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{8}$

$\boxed{\text{z159}}$ $\quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g,a) = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z175}}$ $\quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g,a) = \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z176}}$ $\quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g,b) = -\dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$

$\boxed{\text{z177}}$ $\quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g,b) = \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{1g})}{2}$

$\boxed{\text{z206}}$ $\quad \mathbb{Q}_{1,1}^{(c)}(E_u) = -\dfrac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z207}}$ $\quad \mathbb{Q}_{1,2}^{(c)}(E_u) = \dfrac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z208}}$ $\quad \mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\dfrac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z209}}$ $\quad \mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \dfrac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z210}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,1) = -\dfrac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z211}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,1) = -\dfrac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z212}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,2) = \dfrac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z213}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,2) = -\dfrac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

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

$\boxed{\text{z10}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z52}}$ $\mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \dfrac{\sqrt{3}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \dfrac{\sqrt{3}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} + \dfrac{\sqrt{3}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$

$\boxed{\text{z77}}$ $\mathbb{G}_2^{(1,-1;c)}(A_{1u}) = -\dfrac{\sqrt{6}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{6} + \dfrac{\sqrt{6}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{6} + \dfrac{\sqrt{6}\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$

$\boxed{\text{z78}}$ $\mathbb{Q}_1^{(1,-1;c)}(A_{2u}) = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} + \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z120}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{1u}) = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2} + \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z121}}$ $\mathbb{Q}_2^{(c)}(B_{2g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{2g})$

$\boxed{\text{z143}}$ $\mathbb{Q}_3^{(1,-1;c)}(B_{2u}) = \mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{M}_2^{(b)}(B_{1u})$

$\boxed{\text{z160}}$ $\mathbb{G}_2^{(1,-1;c)}(B_{2u}) = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z178}}$ $\mathbb{Q}_{2,1}^{(c)}(E_g) = \dfrac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

12

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

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

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

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

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

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

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

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

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

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

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

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

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

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

13

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$\boxed{\text{z222}}$ $\mathbb{Q}_{1,1}^{(c)}(E_u, b) = \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$

$\boxed{\text{z223}}$ $\mathbb{Q}_{1,2}^{(c)}(E_u, b) = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2}$

$\boxed{\text{z224}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\dfrac{\sqrt{30}\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \dfrac{\sqrt{10}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \dfrac{\sqrt{10}\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10}$

$\boxed{\text{z225}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u) = \dfrac{\sqrt{30}\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \dfrac{\sqrt{10}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \dfrac{\sqrt{10}\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10}$

$\boxed{\text{z226}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 1) = \dfrac{\sqrt{30}\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} + \dfrac{\sqrt{10}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} + \dfrac{\sqrt{10}\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{5}$

$\boxed{\text{z227}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 1) = -\dfrac{\sqrt{30}\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{20} + \dfrac{\sqrt{10}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{20} - \dfrac{\sqrt{10}\mathbb{G}_2^{(1,-1;a)}(B_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{5}$

$\boxed{\text{z228}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 2) = \dfrac{\sqrt{2}\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \dfrac{\sqrt{6}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4}$

$\boxed{\text{z229}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 2) = -\dfrac{\sqrt{2}\mathbb{G}_2^{(1,-1;a)}(A_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \dfrac{\sqrt{6}\mathbb{G}_2^{(1,-1;a)}(B_{1u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4}$

$\boxed{\text{z230}}$ $\mathbb{Q}_{1,1}^{(1,0;c)}(E_u, a) = \dfrac{\sqrt{2}\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z231}}$ $\mathbb{Q}_{1,2}^{(1,0;c)}(E_u, a) = \dfrac{\sqrt{2}\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$

$\boxed{\text{z232}}$ $\mathbb{Q}_{1,1}^{(1,0;c)}(E_u, b) = \dfrac{\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2} + \dfrac{\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z233}}$ $\mathbb{Q}_{1,2}^{(1,0;c)}(E_u, b) = \dfrac{\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2} + \dfrac{\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z234}}$ $\mathbb{Q}_{3,1}^{(1,0;c)}(E_u, 2) = \dfrac{\mathbb{Q}_{1,2}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2} - \dfrac{\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z235}}$ $\mathbb{Q}_{3,2}^{(1,0;c)}(E_u, 2) = \dfrac{\mathbb{Q}_{1,1}^{(1,0;a)}(E_u)\mathbb{Q}_2^{(b)}(B_{2g})}{2} - \dfrac{\mathbb{Q}_1^{(1,0;a)}(A_{2u})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

17

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{z101}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{1u}) = -\frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{3} - \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

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

$$\boxed{\text{z103}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{1u},b) = \frac{3\sqrt{7}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} - \frac{\sqrt{105}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{42} + \frac{3\sqrt{7}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{14}$$
$$- \frac{\sqrt{105}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{42} + \frac{\sqrt{105}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{21}$$

$$\boxed{\text{z104}} \quad \mathbb{G}_4^{(1,-1;c)}(B_{1u}) = \frac{\sqrt{35}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{14} + \frac{\sqrt{35}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{14} + \frac{\sqrt{21}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{14} - \frac{\sqrt{21}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(A_{2u})}{7}$$

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

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

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

$$\boxed{\text{z127}} \quad \mathbb{Q}_4^{(1,-1;c)}(B_{2g}) = \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} + \frac{\sqrt{15}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_2^{(b)}(B_{2g})}{5}$$

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

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

$$\boxed{\text{z130}} \quad \mathbb{Q}_3^{(1,-1;c)}(B_{2u},b) = \frac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{4} + \frac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{12} - \frac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \frac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{12} + \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{3}$$

$$\boxed{\text{z131}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u},a) = \frac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_{1,2}^{(b)}(E_u)}{2} - \frac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$$

$$\boxed{\text{z148}} \quad \mathbb{G}_2^{(1,-1;c)}(B_{2u},b) = -\frac{\sqrt{7}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{7} + \frac{\sqrt{105}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{21} + \frac{\sqrt{7}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{7}$$
$$- \frac{\sqrt{105}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{21} + \frac{\sqrt{105}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{21}$$

$$\boxed{\text{z149}} \quad \mathbb{G}_4^{(1,-1;c)}(B_{2u}) = -\frac{\sqrt{35}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,2}^{(b)}(E_u)}{28} - \frac{3\sqrt{21}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,2}^{(b)}(E_u)}{28} + \frac{\sqrt{35}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_{1,1}^{(b)}(E_u)}{28} + \frac{3\sqrt{21}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_{1,1}^{(b)}(E_u)}{28} + \frac{\sqrt{21}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_1^{(b)}(A_{2u})}{7}$$

$$\boxed{\text{z150}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g,a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z151}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g,a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z165}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g,b) = -\frac{\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z166}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g,b) = \frac{\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} + \frac{\mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z167}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g,1) = -\frac{\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z168}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g,1) = \frac{\mathbb{Q}_2^{(a)}(B_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\mathbb{Q}_2^{(a)}(B_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z184}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g,a) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z185}} \quad \mathbb{Q}_{2,2}^{(1,-1;c)}(E_g,a) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z186}} \quad \mathbb{Q}_{2,1}^{(1,-1;c)}(E_g,b) = \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{2g})}{4} + \frac{\sqrt{2}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4}$$

$\boxed{\text{z187}}$ $\mathbb{Q}_{2,2}^{(1,-1;c)}(E_g, b) = \dfrac{\sqrt{6}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{2g})}{4} + \dfrac{\sqrt{2}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4}$

$\boxed{\text{z188}}$ $\mathbb{Q}_{4,1}^{(1,-1;c)}(E_g, 1) = \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{2g})}{4} - \dfrac{\sqrt{6}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4}$

$\boxed{\text{z189}}$ $\mathbb{Q}_{4,2}^{(1,-1;c)}(E_g, 1) = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(1,-1;a)}(E_g)\mathbb{Q}_2^{(b)}(B_{2g})}{4} - \dfrac{\sqrt{6}\mathbb{Q}_2^{(1,-1;a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4}$

$\boxed{\text{z236}}$ $\mathbb{Q}_{1,1}^{(c)}(E_u) = -\dfrac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z237}}$ $\mathbb{Q}_{1,2}^{(c)}(E_u) = \dfrac{\sqrt{2}\mathbb{M}_1^{(a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z238}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u, a) = -\dfrac{\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \dfrac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z239}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u, a) = -\dfrac{\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \dfrac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z240}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u, b) = \dfrac{\sqrt{2}\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{1u})}{2}$

$\boxed{\text{z241}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u, b) = \dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{M}_2^{(b)}(B_{1u})}{2}$

$\boxed{\text{z242}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u, c) = \dfrac{3\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{M}_2^{(b)}(B_{1u})}{8} - \dfrac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{M}_2^{(b)}(B_{1u})}{8}$

$\boxed{\text{z243}}$ $\mathbb{Q}_{1,2}^{(1,-1;c)}(E_u, c) = \dfrac{3\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{M}_2^{(b)}(B_{1u})}{8} - \dfrac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{M}_2^{(b)}(B_{1u})}{8}$

$\boxed{\text{z244}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 1a) = \dfrac{\sqrt{78}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{26} - \dfrac{\sqrt{130}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{26} - \dfrac{\sqrt{130}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{26}$

$\boxed{\text{z245}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u, 1a) = \dfrac{\sqrt{78}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{T}_1^{(b)}(A_{2u})}{26} - \dfrac{\sqrt{130}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{T}_1^{(b)}(A_{2u})}{26} - \dfrac{\sqrt{130}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{26}$

$\boxed{\text{z246}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u, 1b) = \dfrac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 1)\mathbb{M}_2^{(b)}(B_{1u})}{8} + \dfrac{3\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g, 2)\mathbb{M}_2^{(b)}(B_{1u})}{8}$

$\boxed{\text{z247}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,1b) = \dfrac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{M}_2^{(b)}(B_{1u})}{8} + \dfrac{3\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{M}_2^{(b)}(B_{1u})}{8}$

$\boxed{\text{z248}}$ $\mathbb{Q}_{3,1}^{(1,-1;c)}(E_u,2) = -\dfrac{5\sqrt{65}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{104} - \dfrac{\sqrt{39}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{312} + \dfrac{\sqrt{39}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{12} - \dfrac{7\sqrt{39}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{156}$

$\boxed{\text{z249}}$ $\mathbb{Q}_{3,2}^{(1,-1;c)}(E_u,2) = -\dfrac{5\sqrt{65}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{104} - \dfrac{\sqrt{39}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{312} - \dfrac{\sqrt{39}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{12} - \dfrac{7\sqrt{39}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{156}$

$\boxed{\text{z250}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E_u,a) = -\dfrac{\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} + \dfrac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{2}$

$\boxed{\text{z251}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E_u,a) = -\dfrac{\mathbb{M}_{1,1}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2} - \dfrac{\mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{2}$

$\boxed{\text{z252}}$ $\mathbb{G}_{2,1}^{(1,-1;c)}(E_u,b) = \dfrac{\sqrt{10}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \dfrac{5\sqrt{6}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{24} + \dfrac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{12} - \dfrac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{12}$

$\boxed{\text{z253}}$ $\mathbb{G}_{2,2}^{(1,-1;c)}(E_u,b) = \dfrac{\sqrt{10}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \dfrac{5\sqrt{6}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{24} - \dfrac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{12} - \dfrac{\sqrt{6}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{12}$

$\boxed{\text{z254}}$ $\mathbb{G}_{4,1}^{(1,-1;c)}(E_u,1) = -\dfrac{\sqrt{5}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \dfrac{\sqrt{3}\mathbb{M}_{3,2}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{8} - \dfrac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4} - \dfrac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4}$

$\boxed{\text{z255}}$ $\mathbb{G}_{4,2}^{(1,-1;c)}(E_u,1) = -\dfrac{\sqrt{5}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,1)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \dfrac{\sqrt{3}\mathbb{M}_{3,1}^{(1,-1;a)}(E_g,2)\mathbb{T}_1^{(b)}(A_{2u})}{8} + \dfrac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{1g})\mathbb{T}_{1,2}^{(b)}(E_u)}{4} - \dfrac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{2g})\mathbb{T}_{1,1}^{(b)}(E_u)}{4}$

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

$\boxed{\text{z19}}$ $\mathbb{Q}_0^{(c)}(A_{1g}) = \mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_0^{(b)}(A_{1g})$

$\boxed{\text{z132}}$ $\mathbb{G}_0^{(1,-1;c)}(A_{1u}) = \mathbb{M}_1^{(1,-1;a)}(A_{2g})\mathbb{T}_1^{(b)}(A_{2u})$

$\boxed{\text{z256}}$ $\mathbb{Q}_{1,1}^{(1,-1;c)}(E_u) = -\dfrac{\sqrt{2}\mathbb{M}_{1,2}^{(1,-1;a)}(E_g)\mathbb{T}_1^{(b)}(A_{2u})}{2}$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

24

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

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

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

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

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

— Atomic SAMB

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$\boxed{\text{x21}}$ $\mathbb{Q}_0^{(a)}(A_{1g}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$

$\boxed{\text{x22}}$ $\mathbb{Q}_2^{(a)}(B_{1g}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$

$\boxed{\text{x23}}$ $\mathbb{Q}_2^{(a)}(B_{2g}) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{bmatrix}$

$\boxed{\text{x24}}$ $\mathbb{Q}_2^{(1,-1;a)}(A_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & \frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 \end{bmatrix}$

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

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

$\boxed{\text{x27}}$ $\mathbb{M}_1^{(a)}(A_{2g}) = \begin{bmatrix} 0 & 0 & -\frac{i}{2} & 0 \\ 0 & 0 & 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 & 0 & 0 \\ 0 & \frac{i}{2} & 0 & 0 \end{bmatrix}$

$$\boxed{\text{x28}} \quad \mathbb{M}_1^{(1,-1;a)}(A_{2g}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \end{bmatrix}$$

$$\boxed{\text{x29}} \quad \mathbb{M}_3^{(1,-1;a)}(B_{1g}) = \begin{bmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x30}} \quad \mathbb{M}_3^{(1,-1;a)}(B_{2g}) = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

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

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

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

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

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

28

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`

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

- Bond cluster

** Wyckoff: `2a@2b`

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

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

** Wyckoff: `4b@4c`

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

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

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

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

** Wyckoff: `8a@8f`

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

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

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

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

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

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

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

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

━━ **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 (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, $|v| = 1.0$ (cartesian)

SL	vector (v)	center (c)	mapping	head	tail	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, $|v| = 1.35853$ (cartesian)

SL	vector (v)	center (c)	mapping	head	tail	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]