Model for “D2h1”

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

Group and Unit Cell

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

Symmetry Operation

Table 1: Symmetry operation

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

Harmonics

Table 2: Harmonics

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

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
9	$\mathbb{G}_4(A_u,1)$	A_u	4	G, M	1	-	$\frac{\sqrt{21}\left(x^4-3x^2y^2-3x^2z^2+y^4-3y^2z^2+z^4\right)}{6}$
10	$\mathbb{G}_1(B_{1g})$	B_{1g}	1	G, M	-	-	z
11	$\mathbb{Q}_2(B_{1g})$	B_{1g}	2	Q, T	-	-	$\sqrt{3}xy$
12	$\mathbb{G}_3(B_{1g},1)$	B_{1g}	3	G, M	1	-	$-\frac{z\left(3x^2+3y^2-2z^2\right)}{2}$
13	$\mathbb{G}_3(B_{1g},2)$	B_{1g}	3	G, M	2	-	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
14	$\mathbb{Q}_4(B_{1g},1)$	B_{1g}	4	Q, T	1	-	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
15	$\mathbb{Q}_1(B_{1u})$	B_{1u}	1	Q, T	-	-	z
16	$\mathbb{G}_2(B_{1u})$	B_{1u}	2	G, M	-	-	$\sqrt{3}xy$
17	$\mathbb{Q}_3(B_{1u},1)$	B_{1u}	3	Q, T	1	-	$-\frac{z\left(3x^2+3y^2-2z^2\right)}{2}$
18	$\mathbb{Q}_3(B_{1u},2)$	B_{1u}	3	Q, T	2	-	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
19	$\mathbb{G}_4(B_{1u},1)$	B_{1u}	4	G, M	1	-	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
20	$\mathbb{G}_1(B_{2g})$	B_{2g}	1	G, M	-	-	y
21	$\mathbb{Q}_2(B_{2g})$	B_{2g}	2	Q, T	-	-	$\sqrt{3}xz$
22	$\mathbb{G}_3(B_{2g},1)$	B_{2g}	3	G, M	1	-	$-\frac{y\left(3x^2-2y^2+3z^2\right)}{2}$
23	$\mathbb{G}_3(B_{2g},2)$	B_{2g}	3	G, M	2	-	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
24	$\mathbb{Q}_1(B_{2u})$	B_{2u}	1	Q, T	-	-	y
25	$\mathbb{G}_2(B_{2u})$	B_{2u}	2	G, M	-	-	$\sqrt{3}xz$
26	$\mathbb{Q}_3(B_{2u},1)$	B_{2u}	3	Q, T	1	-	$-\frac{y\left(3x^2-2y^2+3z^2\right)}{2}$
27	$\mathbb{Q}_3(B_{2u},2)$	B_{2u}	3	Q, T	2	-	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
28	$\mathbb{G}_1(B_{3g})$	B_{3g}	1	G, M	-	-	x
29	$\mathbb{Q}_2(B_{3g})$	B_{3g}	2	Q, T	-	-	$\sqrt{3}yz$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
30	$\mathbb{G}_3(B_{3g},1)$	B_{3g}	3	$G,\ M$	1	-	$\frac{x(2x^2-3y^2-3z^2)}{2}$
31	$\mathbb{G}_3(B_{3g},2)$	B_{3g}	3	$G,\ M$	2	-	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
32	$\mathbb{Q}_1(B_{3u})$	B_{3u}	1	$Q,\ T$	-	-	x
33	$\mathbb{G}_2(B_{3u})$	B_{3u}	2	$G,\ M$	-	-	$\sqrt{3}yz$
34	$\mathbb{Q}_3(B_{3u},1)$	B_{3u}	3	$Q,\ T$	1	-	$\frac{x(2x^2-3y^2-3z^2)}{2}$
35	$\mathbb{Q}_3(B_{3u},2)$	B_{3u}	3	$Q,\ T$	2	-	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$

Basis in full matrix

Table 3: dimension = 8

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

Table 4: Atomic basis (orbital part only)

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

SAMB

348 (all 348) SAMBs

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

* wyckoff: `2d@1f`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 'A'-'A' bond-cluster : `A;A_004_1`
  * bra: $\langle p_x, \uparrow|$, $\langle p_x, \downarrow|$, $\langle p_y, \uparrow|$, $\langle p_y, \downarrow|$, $\langle p_z, \uparrow|$, $\langle p_z, \downarrow|$

* ket: $|p_x,\uparrow\rangle$, $|p_x,\downarrow\rangle$, $|p_y,\uparrow\rangle$, $|p_y,\downarrow\rangle$, $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$
* wyckoff: `2d@1f`

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

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

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

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

$\boxed{\text{z49}}$ $\mathbb{Q}_0^{(1,-1;c)}(A_g)=\mathbb{Q}_2^{(1,-1;a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z50}}$ $\mathbb{Q}_2^{(1,-1;c)}(A_g,1)=\mathbb{Q}_2^{(1,-1;a)}(A_g,1)\mathbb{Q}_0^{(b)}(A_g)$

$\boxed{\text{z51}}$ $\mathbb{Q}_2^{(1,-1;c)}(A_g,2)=\mathbb{Q}_2^{(1,-1;a)}(A_g,2)\mathbb{Q}_0^{(b)}(A_g)$

$\boxed{\text{z52}}$ $\mathbb{Q}_2^{(1,0;c)}(A_g,2)=-\mathbb{G}_1^{(1,0;a)}(B_{1g})\mathbb{Q}_2^{(b)}(B_{1g})$

$\boxed{\text{z53}}$ $\mathbb{Q}_0^{(1,1;c)}(A_g)=\mathbb{Q}_0^{(1,1;a)}(A_g)\mathbb{Q}_0^{(b)}(A_g)$

$\boxed{\text{z82}}$ $\mathbb{Q}_3^{(1,-1;c)}(A_u)=-\frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{2g},2)\mathbb{T}_1^{(b)}(B_{2u})}{2}-\frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{3g},2)\mathbb{T}_1^{(b)}(B_{3u})}{2}$

$\boxed{\text{z83}}$ $\mathbb{Q}_3^{(1,0;c)}(A_u)=\frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2}+\frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$

$\boxed{\text{z84}}$ $\mathbb{G}_0^{(c)}(A_u)=\frac{\sqrt{2}\mathbb{M}_1^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2}+\frac{\sqrt{2}\mathbb{M}_1^{(a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$

$\boxed{\text{z85}}$ $\mathbb{G}_2^{(c)}(A_u,2)=-\frac{\sqrt{2}\mathbb{M}_1^{(a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2}+\frac{\sqrt{2}\mathbb{M}_1^{(a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$

$\boxed{\text{z86}}$ $\mathbb{G}_0^{(1,-1;c)}(A_u)=\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2}+\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$

$\boxed{\text{z87}}$ $\mathbb{G}_2^{(1,-1;c)}(A_u,1)=-\frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{2g},1)\mathbb{T}_1^{(b)}(B_{2u})}{4}+\frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{2g},2)\mathbb{T}_1^{(b)}(B_{2u})}{4}-\frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{3g},1)\mathbb{T}_1^{(b)}(B_{3u})}{4}-\frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{3g},2)\mathbb{T}_1^{(b)}(B_{3u})}{4}$

$\boxed{\text{z88}}$ $\mathbb{G}_2^{(1,-1;c)}(A_u,2a) = -\frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{2g},1)\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_3^{(1,-1;a)}(B_{3g},1)\mathbb{T}_1^{(b)}(B_{3u})}{2}$

$\boxed{\text{z89}}$ $\mathbb{G}_2^{(1,-1;c)}(A_u,2b) = -\frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2} + \frac{\sqrt{2}\mathbb{M}_1^{(1,-1;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$

$\boxed{\text{z90}}$ $\mathbb{G}_4^{(1,-1;c)}(A_u,1) = \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{2g},1)\mathbb{T}_1^{(b)}(B_{2u})}{4} + \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{2g},2)\mathbb{T}_1^{(b)}(B_{2u})}{4} + \frac{\sqrt{5}\mathbb{M}_3^{(1,-1;a)}(B_{3g},1)\mathbb{T}_1^{(b)}(B_{3u})}{4} - \frac{\sqrt{3}\mathbb{M}_3^{(1,-1;a)}(B_{3g},2)\mathbb{T}_1^{(b)}(B_{3u})}{4}$

$\boxed{\text{z118}}$ $\mathbb{G}_2^{(1,0;c)}(A_u,1) = \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{2g})\mathbb{T}_1^{(b)}(B_{2u})}{2} - \frac{\sqrt{2}\mathbb{T}_2^{(1,0;a)}(B_{3g})\mathbb{T}_1^{(b)}(B_{3u})}{2}$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Atomic SAMB

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$\boxed{\text{x62}}$ $$\mathbb{T}_{2}^{(1,0;a)}(B_{1g})=\begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{6} & 0 & 0 & -\frac{\sqrt{6}i}{12} \\ 0 & 0 & 0 & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}i}{12} & 0 \\ 0 & -\frac{\sqrt{6}}{12} & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 \\ -\frac{\sqrt{6}}{12} & 0 & \frac{\sqrt{6}i}{12} & 0 & 0 & 0 \end{bmatrix}$$

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

$\boxed{\text{x64}}$ $$\mathbb{T}_{2}^{(1,0;a)}(B_{3g})=\begin{bmatrix} 0 & 0 & 0 & \frac{\sqrt{6}i}{12} & \frac{\sqrt{6}}{12} & 0 \\ 0 & 0 & -\frac{\sqrt{6}i}{12} & 0 & 0 & -\frac{\sqrt{6}}{12} \\ 0 & \frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 \\ -\frac{\sqrt{6}i}{12} & 0 & \frac{\sqrt{6}}{6} & 0 & 0 & 0 \\ \frac{\sqrt{6}}{12} & 0 & 0 & 0 & 0 & -\frac{\sqrt{6}}{6} \\ 0 & -\frac{\sqrt{6}}{12} & 0 & 0 & -\frac{\sqrt{6}}{6} & 0 \end{bmatrix}$$

Cluster SAMB

- Site cluster

** Wyckoff: `1a`

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

- Bond cluster

** Wyckoff: `1c@1b`

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

$\boxed{\text{y3}}$ $\mathbb{T}_1^{(s)}(B_{3u}) = [i]$

** Wyckoff: `1a@1c`

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

$\boxed{\text{y5}}$ $\mathbb{T}_1^{(s)}(B_{1u}) = [i]$

** Wyckoff: `1b@1e`

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

$\boxed{\text{y7}}$ $\mathbb{T}_1^{(s)}(B_{2u}) = [i]$

** Wyckoff: `2d@1f`

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

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

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

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

Site and Bond

Table 5: Orbital of each site

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

Table 6: Neighbor and bra-ket of each bond

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

Site in Unit Cell

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

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

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

Bond in Unit Cell

Bonds in (conventional) cell (no plus set): tail, head = (SL, plus set), (N)D = (non)directional (listed up to 5th neighbor at most)

Table 8: 1-th 'A'-'A' [1] (#1) bond cluster (1c@1b), ND, $|\boldsymbol{v}|$= 1.0 (cartesian)

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

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

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

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

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

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

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