

# Model for “SrVO3”

Generated on 2026-01-26 01:23:07 by MultiPie 2.0.6

---

## General Condition

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

---

## Group and Unit Cell

- Group: SG No. 221  $O_h^1 Pm\bar{3}m$  [ cubic ]
- Associated point group: PG No. 221  $O_h m\bar{3}m$  [ cubic ]
- Unit cell:
  - $a = 3.84090$ ,  $b = 3.84090$ ,  $c = 3.84090$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 90.0$
- Lattice vectors (conventional cell):
  - $\mathbf{a}_1 = [ 3.84090, 0.00000, 0.00000 ]$
  - $\mathbf{a}_2 = [ 0.00000, 3.84090, 0.00000 ]$
  - $\mathbf{a}_3 = [ 0.00000, 0.00000, 3.84090 ]$

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	$\{3_{111}^+ 0\}$
6	$\{3_{-11-1}^+ 0\}$	7	$\{3_{1-1-1}^+ 0\}$	8	$\{3_{-1-11}^+ 0\}$	9	$\{3_{111}^- 0\}$	10	$\{3_{1-1-1}^- 0\}$
11	$\{3_{-1-11}^- 0\}$	12	$\{3_{-11-1}^- 0\}$	13	$\{2_{110} 0\}$	14	$\{2_{1-10} 0\}$	15	$\{4_{001}^- 0\}$
16	$\{4_{001}^+ 0\}$	17	$\{4_{100}^- 0\}$	18	$\{2_{011} 0\}$	19	$\{2_{01-1} 0\}$	20	$\{4_{100}^+ 0\}$
21	$\{4_{010}^+ 0\}$	22	$\{2_{101} 0\}$	23	$\{4_{010}^- 0\}$	24	$\{2_{-101} 0\}$	25	$\{-1 0\}$
26	$\{m_{001} 0\}$	27	$\{m_{010} 0\}$	28	$\{m_{100} 0\}$	29	$\{-3_{111}^+ 0\}$	30	$\{-3_{-11-1}^+ 0\}$
31	$\{-3_{1-1-1}^+ 0\}$	32	$\{-3_{-1-11}^+ 0\}$	33	$\{-3_{111}^- 0\}$	34	$\{-3_{1-1-1}^- 0\}$	35	$\{-3_{-1-11}^- 0\}$
36	$\{-3_{-11-1}^- 0\}$	37	$\{m_{110} 0\}$	38	$\{m_{1-10} 0\}$	39	$\{-4_{001}^- 0\}$	40	$\{-4_{001}^+ 0\}$
41	$\{-4_{100}^- 0\}$	42	$\{m_{011} 0\}$	43	$\{m_{01-1} 0\}$	44	$\{-4_{100}^+ 0\}$	45	$\{-4_{010}^+ 0\}$
46	$\{m_{101} 0\}$	47	$\{-4_{010}^- 0\}$	48	$\{m_{-101} 0\}$				

Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A_{1g})$	$A_{1g}$	0	$Q, T$	-	-	1
2	$\mathbb{Q}_4(A_{1g})$	$A_{1g}$	4	$Q, T$	-	-	$\frac{\sqrt{21}(x^4-3x^2y^2-3x^2z^2+y^4-3y^2z^2+z^4)}{6}$
3	$\mathbb{G}_0(A_{1u})$	$A_{1u}$	0	$G, M$	-	-	1
4	$\mathbb{G}_3(A_{2g})$	$A_{2g}$	3	$G, M$	-	-	$\sqrt{15}xyz$
5	$\mathbb{Q}_3(A_{2u})$	$A_{2u}$	3	$Q, T$	-	-	$\sqrt{15}xyz$
6	$\mathbb{Q}_{2,1}(E_g)$	$E_g$	2	$Q, T$	-	1	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
7	$\mathbb{Q}_{2,2}(E_g)$					2	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
8	$\mathbb{Q}_{4,1}(E_g)$	$E_g$	4	$Q, T$	-	1	$-\frac{\sqrt{15}(x^4-12x^2y^2+6x^2z^2+y^4+6y^2z^2-2z^4)}{12}$
9	$\mathbb{Q}_{4,2}(E_g)$					2	$\frac{\sqrt{5}(x-y)(x+y)(x^2+y^2-6z^2)}{4}$
10	$\mathbb{G}_{2,1}(E_u)$	$E_u$	2	$G, M$	-	1	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
11	$\mathbb{G}_{2,2}(E_u)$					2	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
12	$\mathbb{G}_{1,1}(T_{1g})$	$T_{1g}$	1	$G, M$	-	1	$x$
13	$\mathbb{G}_{1,2}(T_{1g})$					2	$y$
14	$\mathbb{G}_{1,3}(T_{1g})$					3	$z$
15	$\mathbb{G}_{3,1}(T_{1g})$	$T_{1g}$	3	$G, M$	-	1	$\frac{x(2x^2-3y^2-3z^2)}{2}$
16	$\mathbb{G}_{3,2}(T_{1g})$					2	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
17	$\mathbb{G}_{3,3}(T_{1g})$					3	$-\frac{z(3x^2+3y^2-2z^2)}{2}$
18	$\mathbb{Q}_{4,1}(T_{1g})$	$T_{1g}$	4	$Q, T$	-	1	$\frac{\sqrt{35}yz(y-z)(y+z)}{2}$
19	$\mathbb{Q}_{4,2}(T_{1g})$					2	$-\frac{\sqrt{35}xz(x-z)(x+z)}{2}$
20	$\mathbb{Q}_{4,3}(T_{1g})$					3	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
21	$\mathbb{Q}_{1,1}(T_{1u})$	$T_{1u}$	1	$Q, T$	-	1	$x$
22	$\mathbb{Q}_{1,2}(T_{1u})$					2	$y$
23	$\mathbb{Q}_{1,3}(T_{1u})$					3	$z$
24	$\mathbb{Q}_{2,1}(T_{2g})$	$T_{2g}$	2	$Q, T$	-	1	$\sqrt{3}yz$
25	$\mathbb{Q}_{2,2}(T_{2g})$					2	$\sqrt{3}xz$
26	$\mathbb{Q}_{2,3}(T_{2g})$					3	$\sqrt{3}xy$
27	$\mathbb{G}_{3,1}(T_{2g})$	$T_{2g}$	3	$G, M$	-	1	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
28	$\mathbb{G}_{3,2}(T_{2g})$					2	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
29	$\mathbb{G}_{3,3}(T_{2g})$					3	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
30	$\mathbb{Q}_{4,1}(T_{2g})$	$T_{2g}$	4	$Q, T$	-	1	$\frac{\sqrt{5}yz(6x^2-y^2-z^2)}{2}$
31	$\mathbb{Q}_{4,2}(T_{2g})$					2	$-\frac{\sqrt{5}xz(x^2-6y^2+z^2)}{2}$
32	$\mathbb{Q}_{4,3}(T_{2g})$					3	$-\frac{\sqrt{5}xy(x^2+y^2-6z^2)}{2}$
33	$\mathbb{G}_{2,1}(T_{2u})$	$T_{2u}$	2	$G, M$	-	1	$\sqrt{3}yz$
34	$\mathbb{G}_{2,2}(T_{2u})$					2	$\sqrt{3}xz$
35	$\mathbb{G}_{2,3}(T_{2u})$					3	$\sqrt{3}xy$
36	$\mathbb{Q}_{3,1}(T_{2u})$	$T_{2u}$	3	$Q, T$	-	1	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
37	$\mathbb{Q}_{3,2}(T_{2u})$					2	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
38	$\mathbb{Q}_{3,3}(T_{2u})$					3	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$

Table 3: dimension = 3

#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)
0	$ d_{yz}\rangle @V(1)$	1	$ d_{xz}\rangle @V(1)$	2	$ d_{xy}\rangle @V(1)$

Table 4: Atomic basis (orbital part only)

orbital	definition
$ d_u\rangle$	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
$ d_v\rangle$	$\frac{\sqrt{3}(x^2 - y^2)}{2}$
$ d_{yz}\rangle$	$\sqrt{3}yz$
$ d_{xz}\rangle$	$\sqrt{3}xz$
$ d_{xy}\rangle$	$\sqrt{3}xy$

---

**SAMB**


---

87 (all 87) SAMBs

- 'V' site-cluster : V
  - \* bra:  $\langle d_{yz}|, \langle d_{xz}|, \langle d_{xy}|$
  - \* ket:  $|d_{yz}\rangle, |d_{xz}\rangle, |d_{xy}\rangle$
  - \* wyckoff: **1a**

z1

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

$$\boxed{\text{z9}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z10}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(s)}(A_{1g})}{2}$$

$$\boxed{\text{z37}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z38}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

$$\boxed{\text{z39}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_0^{(s)}(A_{1g})}{3}$$

• 'V'-'V' bond-cluster : V;V\_001\_1

\* bra:  $\langle d_{yz} |, \langle d_{xz} |, \langle d_{xy} |$

\* ket:  $|d_{yz}\rangle, |d_{xz}\rangle, |d_{xy}\rangle$

\* wyckoff: 3a@3d

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

$$\boxed{\text{z3}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z7}} \quad \mathbb{G}_0^{(c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z11}} \quad \mathbb{G}_3^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z12}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z13}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z14}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\begin{aligned}
\boxed{\text{z15}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) &= \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2} \\
\boxed{\text{z16}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, c) &= \frac{\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} \\
\boxed{\text{z25}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, c) &= -\frac{\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} \\
\boxed{\text{z26}} \quad \mathbb{G}_{2,1}^{(c)}(E_u) &= -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3} \\
\boxed{\text{z27}} \quad \mathbb{G}_{2,2}^{(c)}(E_u) &= \frac{\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2} \\
\boxed{\text{z40}} \quad \mathbb{Q}_{4,1}^{(c)}(T_{1g}) &= -\frac{\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\boxed{\text{z41}} \quad \mathbb{Q}_{4,2}^{(c)}(T_{1g}) &= \frac{\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\boxed{\text{z42}} \quad \mathbb{Q}_{4,3}^{(c)}(T_{1g}) &= \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{3} \\
\boxed{\text{z43}} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z44}} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z45}} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z61}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z64}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z65}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}
\end{aligned}$$

$$\boxed{\text{z70}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, b) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} - \frac{\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z71}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, b) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6} + \frac{\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z72}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, b) = -\frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{3}$$

$$\boxed{\text{z79}} \quad \mathbb{G}_{2,1}^{(c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z80}} \quad \mathbb{G}_{2,2}^{(c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$$\boxed{\text{z81}} \quad \mathbb{G}_{2,3}^{(c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

• 'V'-'V' bond-cluster : V;V\_002\_1

\* bra:  $\langle d_{yz} |, \langle d_{xz} |, \langle d_{xy} |$

\* ket:  $|d_{yz}\rangle, |d_{xz}\rangle, |d_{xy}\rangle$

\* wyckoff: 6b03c

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

$$\boxed{\text{z5}} \quad \mathbb{Q}_0^{(c)}(A_{1g}, b) = \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{5}$$

$$\boxed{\text{z6}} \quad \mathbb{Q}_4^{(c)}(A_{1g}) = \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15}$$

$$\boxed{\text{z8}} \quad \mathbb{G}_0^{(c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z17}} \quad \mathbb{G}_3^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z18}} \quad \mathbb{Q}_3^{(c)}(A_{2u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$



$$\boxed{\text{z19}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z20}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$$\boxed{\text{z21}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z22}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

$$\boxed{\text{z23}} \quad \mathbb{Q}_{2,1}^{(c)}(E_g, c) = \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} + \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{7}$$

$$\boxed{\text{z24}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, c) = -\frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{7} - \frac{\sqrt{21}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{7} + \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14}$$

$$\boxed{\text{z28}} \quad \mathbb{Q}_{4,1}^{(c)}(E_g) = \frac{\sqrt{21}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} - \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} - \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} + \frac{2\sqrt{21}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21}$$

$$\boxed{\text{z29}} \quad \mathbb{Q}_{4,2}^{(c)}(E_g) = -\frac{\sqrt{21}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{7}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{7} - \frac{\sqrt{21}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} - \frac{\sqrt{7}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{7}$$

$$\boxed{\text{z30}} \quad \mathbb{G}_{2,1}^{(c)}(E_u, a) = -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$$

$$\boxed{\text{z31}} \quad \mathbb{G}_{2,2}^{(c)}(E_u, a) = \frac{\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{2}$$

$$\boxed{\text{z32}} \quad \mathbb{G}_{2,1}^{(c)}(E_u, b) = \frac{\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{2} - \frac{\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{2}$$

$$\boxed{\text{z33}} \quad \mathbb{G}_{2,2}^{(c)}(E_u, b) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{3}$$

$$\boxed{\text{z34}} \quad \mathbb{Q}_{4,1}^{(c)}(T_{1g}) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{4} - \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{12} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{12}$$

$$\boxed{\text{z35}} \quad \mathbb{Q}_{4,2}^{(c)}(T_{1g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{12} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{12}$$

$$\begin{aligned}
\boxed{\text{z36}} \quad \mathbb{Q}_{4,3}^{(c)}(T_{1g}) &= \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6} \\
\boxed{\text{z46}} \quad \mathbb{G}_{1,1}^{(c)}(T_{1g}) &= -\frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} \\
\boxed{\text{z47}} \quad \mathbb{G}_{1,2}^{(c)}(T_{1g}) &= \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} - \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} \\
\boxed{\text{z48}} \quad \mathbb{G}_{1,3}^{(c)}(T_{1g}) &= -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{15} \\
\boxed{\text{z49}} \quad \mathbb{G}_{3,1}^{(c)}(T_{1g}) &= \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{20} - \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} - \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{60} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{60} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z50}} \quad \mathbb{G}_{3,2}^{(c)}(T_{1g}) &= -\frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{20} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{60} + \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{60} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} \\
\boxed{\text{z51}} \quad \mathbb{G}_{3,3}^{(c)}(T_{1g}) &= -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} \\
\boxed{\text{z52}} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}, a) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z53}} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}, a) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z54}} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}, a) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z55}} \quad \mathbb{Q}_{1,1}^{(c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z56}} \quad \mathbb{Q}_{1,2}^{(c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z57}} \quad \mathbb{Q}_{1,3}^{(c)}(T_{1u}, b) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z58}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z59}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3} \\
\boxed{\text{z60}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, a) &= \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3} \\
\boxed{\text{z62}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, b) &= \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z63}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, b) &= \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z66}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, b) &= \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3} \\
\boxed{\text{z67}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, c) &= \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{42} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} - \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} - \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} \\
\boxed{\text{z68}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, c) &= \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{42} + \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{42} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} \\
\boxed{\text{z69}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, c) &= -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} + \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{21} \\
\boxed{\text{z73}} \quad \mathbb{Q}_{4,1}^{(c)}(T_{2g}) &= -\frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{28} - \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} + \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} \\
\boxed{\text{z74}} \quad \mathbb{Q}_{4,2}^{(c)}(T_{2g}) &= -\frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{28} - \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{28} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} \\
\boxed{\text{z75}} \quad \mathbb{Q}_{4,3}^{(c)}(T_{2g}) &= \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{14} \\
\boxed{\text{z76}} \quad \mathbb{G}_{3,1}^{(c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{12} - \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} + \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{4} \\
\boxed{\text{z77}} \quad \mathbb{G}_{3,2}^{(c)}(T_{2g}) &= \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{12} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{12} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{4} \\
\boxed{\text{z78}} \quad \mathbb{G}_{3,3}^{(c)}(T_{2g}) &= -\frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{6}
\end{aligned}$$

$$\begin{aligned}
\boxed{\text{z82}} \quad \mathbb{Q}_{3,1}^{(c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z83}} \quad \mathbb{Q}_{3,2}^{(c)}(T_{2u}) &= -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z84}} \quad \mathbb{Q}_{3,3}^{(c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6} \\
\boxed{\text{z85}} \quad \mathbb{G}_{2,1}^{(c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z86}} \quad \mathbb{G}_{2,2}^{(c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6} \\
\boxed{\text{z87}} \quad \mathbb{G}_{2,3}^{(c)}(T_{2u}) &= \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}
\end{aligned}$$

---

#### Atomic SAMB

---

- bra:  $\langle d_{yz} |, \langle d_{xz} |, \langle d_{xy} |$
- ket:  $|d_{yz}\rangle, |d_{xz}\rangle, |d_{xy}\rangle$

$$\boxed{\text{x1}} \quad \mathbb{Q}_0^{(a)}(A_{1g}) = \begin{bmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$$

$$\boxed{\text{x2}} \quad \mathbb{Q}_{2,1}^{(a)}(E_g) = \begin{bmatrix} \frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & \frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{6}}{3} \end{bmatrix}$$

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

$$\boxed{\text{x4}} \quad \mathbb{Q}_{2,1}^{(a)}(T_{2g}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$$

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

$$\boxed{\text{x6}} \quad \mathbb{Q}_{2,3}^{(a)}(T_{2g}) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

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

$$\boxed{\text{x8}} \quad \mathbb{M}_{1,2}^{(a)}(T_{1g}) = \begin{bmatrix} 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{\text{x9}} \quad \mathbb{M}_{1,3}^{(a)}(T_{1g}) = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{2} & 0 \\ -\frac{\sqrt{2}i}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

---

### Cluster SAMB

---

- Site cluster

\*\* Wyckoff: **1a**

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

- Bond cluster

\*\* Wyckoff: **3a@3d**

$$\boxed{\text{y2}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3} \right]$$

$$\boxed{\text{y3}} \quad \mathbb{Q}_{2,1}^{(s)}(E_g) = \left[ -\frac{\sqrt{6}}{6}, -\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{3} \right]$$

$$\boxed{\text{y4}} \quad \mathbb{Q}_{2,2}^{(s)}(E_g) = \left[ \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}, 0 \right]$$

$$\boxed{\text{y5}} \quad \mathbb{T}_{1,1}^{(s)}(T_{1u}) = [i, 0, 0]$$

$$\boxed{\text{y6}} \quad \mathbb{T}_{1,2}^{(s)}(T_{1u}) = [0, i, 0]$$

$$\boxed{\text{y7}} \quad \mathbb{T}_{1,3}^{(s)}(T_{1u}) = [0, 0, i]$$

\*\* Wyckoff: **6b@3c**

$$\boxed{\text{y8}} \quad \mathbb{Q}_0^{(s)}(A_{1g}) = \left[ \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y9}} \quad \mathbb{Q}_{2,1}^{(s)}(E_g) = \left[ -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3} \right]$$

$$\boxed{\text{y10}} \quad \mathbb{Q}_{2,2}^{(s)}(E_g) = \left[ \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, 0, 0 \right]$$

$$\boxed{\text{y11}} \quad \mathbb{T}_{1,1}^{(s)}(T_{1u}) = \left[ 0, 0, \frac{i}{2}, \frac{i}{2}, \frac{i}{2}, -\frac{i}{2} \right]$$

$$\boxed{\text{y12}} \quad \mathbb{T}_{1,2}^{(s)}(T_{1u}) = \left[ \frac{i}{2}, -\frac{i}{2}, 0, 0, \frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{\text{y13}} \quad \mathbb{T}_{1,3}^{(s)}(T_{1u}) = \left[ \frac{i}{2}, \frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, 0, 0 \right]$$

$$\boxed{\text{y14}} \quad \mathbb{Q}_{2,1}^{(s)}(T_{2g}) = \left[ \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}, 0, 0, 0, 0 \right]$$

$$\boxed{\text{y15}} \quad \mathbb{Q}_{2,2}^{(s)}(T_{2g}) = \left[ 0, 0, \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2}, 0, 0 \right]$$

$$\boxed{\text{y16}} \quad \mathbb{Q}_{2,3}^{(s)}(T_{2g}) = \left[ 0, 0, 0, 0, \frac{\sqrt{2}}{2}, -\frac{\sqrt{2}}{2} \right]$$

$$\boxed{\text{y17}} \quad \mathbb{M}_{2,1}^{(s)}(T_{2u}) = \left[ 0, 0, \frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{\text{y18}} \quad \mathbb{M}_{2,2}^{(s)}(T_{2u}) = \left[ -\frac{i}{2}, \frac{i}{2}, 0, 0, \frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{\text{y19}} \quad \mathbb{M}_{2,3}^{(s)}(T_{2u}) = \left[ \frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, \frac{i}{2}, 0, 0 \right]$$

---

**Site and Bond**


---

Table 5: Orbital of each site

#	site	orbital
1	<b>v</b>	$ d_{yz}\rangle,  d_{xz}\rangle,  d_{xy}\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	<b>v</b>	<b>v</b>	[1,2]	[d]	[d]

---

**Site in Unit Cell**


---

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

Table 7: 'V' (#1) site cluster (1a), m-3m

SL	position ( $\mathbf{s}$ )	mapping
1	[ 0.00000, 0.00000, 0.00000]	[1,2,3,4,...,48]

### 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 'V'-'V' [1] (#1) bond cluster (3a@3d), ND,  $|\mathbf{v}|= 3.8409$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[-1.00000, 0.00000, 0.00000]	[ 0.50000, 0.00000, 0.00000]	[1,-2,-3,4,17,-18,-19,20,-25,26,27,-28,-41,42,43,-44]	(1,1)	(1,1)	[1,0,0]
2	[ 0.00000,-1.00000, 0.00000]	[ 0.00000, 0.50000, 0.00000]	[5,-6,-7,8,13,-14,-15,16,-29,30,31,-32,-37,38,39,-40]	(1,1)	(1,1)	[0,1,0]
3	[ 0.00000, 0.00000,-1.00000]	[ 0.00000, 0.00000, 0.50000]	[9,-10,-11,12,-21,22,23,-24,-33,34,35,-36,45,-46,-47,48]	(1,1)	(1,1)	[0,0,1]

Table 9: 2-th 'V'-'V' [1] (#2) bond cluster (6b@3c), ND,  $|\mathbf{v}|= 5.43185$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[ 0.00000,-1.00000,-1.00000]	[ 0.00000, 0.50000, 0.50000]	[1,-4,18,-19,-25,28,-42,43]	(1,1)	(1,1)	[0,1,1]

*continued ...*



Table 9

SL	vector ( $\boldsymbol{v}$ )	center ( $\boldsymbol{c}$ )	mapping	head	tail	$\boldsymbol{R}$ (primitive)
2	[ 0.00000, 1.00000, -1.00000]	[ 0.00000, 0.50000, 0.50000]	[2, -3, -17, 20, -26, 27, 41, -44]	(1, 1)	(1, 1)	[0, -1, 1]
3	[-1.00000, 0.00000, -1.00000]	[ 0.50000, 0.00000, 0.50000]	[5, -8, -14, 15, -29, 32, 38, -39]	(1, 1)	(1, 1)	[1, 0, 1]
4	[-1.00000, 0.00000, 1.00000]	[ 0.50000, 0.00000, 0.50000]	[6, -7, 13, -16, -30, 31, -37, 40]	(1, 1)	(1, 1)	[1, 0, -1]
5	[-1.00000, -1.00000, 0.00000]	[ 0.50000, 0.50000, 0.00000]	[9, -12, 21, -24, -33, 36, -45, 48]	(1, 1)	(1, 1)	[1, 1, 0]
6	[ 1.00000, -1.00000, 0.00000]	[ 0.50000, 0.50000, 0.00000]	[10, -11, -22, 23, -34, 35, 46, -47]	(1, 1)	(1, 1)	[-1, 1, 0]