Model for "SrVO3"

Generated on 2026-02-01 12:29:21 by MultiPie 2.0.8

General Condition

- Basis type: `lg`
- 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 $O_{\rm h}^1$ $Pm\bar{3}m$ [cubic]
- Associated point group: PG No. 221 $O_{\rm h}$ $m\bar{3}m$ [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):
  $\boldsymbol{a}_1 =$ [3.84090, 0.00000, 0.00000]
  $\boldsymbol{a}_2 =$ [0.00000, 3.84090, 0.00000]
  $\boldsymbol{a}_3 =$ [0.00000, 0.00000, 3.84090]

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	$\{3^{+}_{111}\|0\}$
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	$\{m_{-101}\|0\}$				

Harmonics

Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A_{1g})$	A_{1g}	0	Q, T	-	-	1

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
2	$\mathbb{Q}_4(A_{1g})$	A_{1g}	4	Q, T	-	-	$\frac{\sqrt{21}\left(x^4-3x^2y^2-3x^2z^2+y^4-3y^2z^2+z^4\right)}{6}$
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	$-\frac{\sqrt{15}\left(x^4-12x^2y^2+6x^2z^2+y^4+6y^2z^2-2z^4\right)}{12}$
9	$\mathbb{Q}_{4,2}(E_g)$					2	$\frac{\sqrt{5}(x-y)(x+y)\left(x^2+y^2-6z^2\right)}{4}$
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	$\frac{x\left(2x^2-3y^2-3z^2\right)}{2}$
16	$\mathbb{G}_{3,2}(T_{1g})$					2	$-\frac{y\left(3x^2-2y^2+3z^2\right)}{2}$
17	$\mathbb{G}_{3,3}(T_{1g})$					3	$-\frac{z\left(3x^2+3y^2-2z^2\right)}{2}$
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	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
21	$\mathbb{Q}_{1,1}(T_{1u})$	T_{1u}	1	Q, T	-	1	x
22	$\mathbb{Q}_{1,2}(T_{1u})$					2	y

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
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	$\frac{\sqrt{5}yz\left(6x^{2}-y^{2}-z^{2}\right)}{2}$
31	$\mathbb{Q}_{4,2}(T_{2g})$					2	$-\frac{\sqrt{5}xz\left(x^{2}-6y^{2}+z^{2}\right)}{2}$
32	$\mathbb{Q}_{4,3}(T_{2g})$					3	$-\frac{\sqrt{5}xy\left(x^{2}+y^{2}-6z^{2}\right)}{2}$
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	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$

Basis in full matrix

Table 3: dimension = 3

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

Table 4: Atomic basis (orbital part only)

orbital	definition
$\left\|d_{v}\right\rangle$	$\frac{\sqrt{3}(x^2-y^2)}{2}$
$\left\|d_{xy}\right\rangle$	$\sqrt{3}xy$
$\left\|d_{xz}\right\rangle$	$\sqrt{3}xz$
$\left\|d_{yz}\right\rangle$	$\sqrt{3}yz$
$\left\|d_{u}\right\rangle$	$-\frac{x^2}{2}-\frac{y^2}{2}+z^2$

— SAMB: 87 (all 87)

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

$$\boxed{\text{z1}}\quad \mathbb{Q}_{0}^{(c)}(A_{1g}) = \mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{0}^{(s)}(A_{1g})$$

$$\boxed{\text{z9}}\quad \mathbb{Q}_{2,1}^{(c)}(E_{g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_{g})\mathbb{Q}_{0}^{(s)}(A_{1g})}{2}$$

$\boxed{\text{z10}}$ $\mathbb{Q}_{2,2}^{(c)}(E_g) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{0}^{(s)}(A_{1g})}{2}$

$\boxed{\text{z37}}$ $\mathbb{Q}_{2,1}^{(c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{0}^{(s)}(A_{1g})}{3}$

$\boxed{\text{z38}}$ $\mathbb{Q}_{2,2}^{(c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{0}^{(s)}(A_{1g})}{3}$

$\boxed{\text{z39}}$ $\mathbb{Q}_{2,3}^{(c)}(T_{2g}) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{0}^{(s)}(A_{1g})}{3}$

- `V;V_001_1` : 'V'-'V' bond-cluster
  * bra: $\langle d_{xy}|$, $\langle d_{xz}|$, $\langle d_{yz}|$
  * ket: $|d_{xy}\rangle$, $|d_{xz}\rangle$, $|d_{yz}\rangle$
  * wyckoff: `3a@3d`

$\boxed{\text{z2}}$ $\mathbb{Q}_{0}^{(c)}(A_{1g}, a) = \mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{0}^{(b)}(A_{1g})$

$\boxed{\text{z3}}$ $\mathbb{Q}_{0}^{(c)}(A_{1g}, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z7}}$ $\mathbb{G}_{0}^{(c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$

$\boxed{\text{z11}}$ $\mathbb{G}_{3}^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z12}}$ $\mathbb{Q}_{2,1}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z13}}$ $\mathbb{Q}_{2,2}^{(c)}(E_g, a) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$

$\boxed{\text{z14}}$ $\mathbb{Q}_{2,1}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z15}}$ $\mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$

$\boxed{\text{z16}}$ $\mathbb{Q}^{(c)}_{2,1}(E_g, c) = \frac{\mathbb{Q}^{(a)}_{2,1}(E_g)\mathbb{Q}^{(b)}_{2,1}(E_g)}{2} - \frac{\mathbb{Q}^{(a)}_{2,2}(E_g)\mathbb{Q}^{(b)}_{2,2}(E_g)}{2}$

$\boxed{\text{z25}}$ $\mathbb{Q}^{(c)}_{2,2}(E_g, c) = -\frac{\mathbb{Q}^{(a)}_{2,1}(E_g)\mathbb{Q}^{(b)}_{2,2}(E_g)}{2} - \frac{\mathbb{Q}^{(a)}_{2,2}(E_g)\mathbb{Q}^{(b)}_{2,1}(E_g)}{2}$

$\boxed{\text{z26}}$ $\mathbb{G}^{(c)}_{2,1}(E_u) = -\frac{\sqrt{3}\mathbb{M}^{(a)}_{1,1}(T_{1g})\mathbb{T}^{(b)}_{1,1}(T_{1u})}{6} - \frac{\sqrt{3}\mathbb{M}^{(a)}_{1,2}(T_{1g})\mathbb{T}^{(b)}_{1,2}(T_{1u})}{6} + \frac{\sqrt{3}\mathbb{M}^{(a)}_{1,3}(T_{1g})\mathbb{T}^{(b)}_{1,3}(T_{1u})}{3}$

$\boxed{\text{z27}}$ $\mathbb{G}^{(c)}_{2,2}(E_u) = \frac{\mathbb{M}^{(a)}_{1,1}(T_{1g})\mathbb{T}^{(b)}_{1,1}(T_{1u})}{2} - \frac{\mathbb{M}^{(a)}_{1,2}(T_{1g})\mathbb{T}^{(b)}_{1,2}(T_{1u})}{2}$

$\boxed{\text{z40}}$ $\mathbb{Q}^{(c)}_{4,1}(T_{1g}) = -\frac{\mathbb{Q}^{(a)}_{2,1}(T_{2g})\mathbb{Q}^{(b)}_{2,1}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}^{(a)}_{2,1}(T_{2g})\mathbb{Q}^{(b)}_{2,2}(E_g)}{6}$

$\boxed{\text{z41}}$ $\mathbb{Q}^{(c)}_{4,2}(T_{1g}) = \frac{\mathbb{Q}^{(a)}_{2,2}(T_{2g})\mathbb{Q}^{(b)}_{2,1}(E_g)}{2} - \frac{\sqrt{3}\mathbb{Q}^{(a)}_{2,2}(T_{2g})\mathbb{Q}^{(b)}_{2,2}(E_g)}{6}$

$\boxed{\text{z42}}$ $\mathbb{Q}^{(c)}_{4,3}(T_{1g}) = \frac{\sqrt{3}\mathbb{Q}^{(a)}_{2,3}(T_{2g})\mathbb{Q}^{(b)}_{2,2}(E_g)}{3}$

$\boxed{\text{z43}}$ $\mathbb{Q}^{(c)}_{1,1}(T_{1u}) = \frac{\sqrt{6}\mathbb{M}^{(a)}_{1,2}(T_{1g})\mathbb{T}^{(b)}_{1,3}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}^{(a)}_{1,3}(T_{1g})\mathbb{T}^{(b)}_{1,2}(T_{1u})}{6}$

$\boxed{\text{z44}}$ $\mathbb{Q}^{(c)}_{1,2}(T_{1u}) = -\frac{\sqrt{6}\mathbb{M}^{(a)}_{1,1}(T_{1g})\mathbb{T}^{(b)}_{1,3}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}^{(a)}_{1,3}(T_{1g})\mathbb{T}^{(b)}_{1,1}(T_{1u})}{6}$

$\boxed{\text{z45}}$ $\mathbb{Q}^{(c)}_{1,3}(T_{1u}) = \frac{\sqrt{6}\mathbb{M}^{(a)}_{1,1}(T_{1g})\mathbb{T}^{(b)}_{1,2}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}^{(a)}_{1,2}(T_{1g})\mathbb{T}^{(b)}_{1,1}(T_{1u})}{6}$

$\boxed{\text{z61}}$ $\mathbb{Q}^{(c)}_{2,1}(T_{2g}, a) = \frac{\sqrt{3}\mathbb{Q}^{(a)}_{2,1}(T_{2g})\mathbb{Q}^{(b)}_{0}(A_{1g})}{3}$

$\boxed{\text{z64}}$ $\mathbb{Q}^{(c)}_{2,2}(T_{2g}, a) = \frac{\sqrt{3}\mathbb{Q}^{(a)}_{2,2}(T_{2g})\mathbb{Q}^{(b)}_{0}(A_{1g})}{3}$

$\boxed{\text{z65}}$ $\mathbb{Q}^{(c)}_{2,3}(T_{2g}, a) = \frac{\sqrt{3}\mathbb{Q}^{(a)}_{2,3}(T_{2g})\mathbb{Q}^{(b)}_{0}(A_{1g})}{3}$

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

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

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

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

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

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

- `V;V_002_1` : 'V'-'V' bond-cluster
  * bra: $\langle d_{xy}|$, $\langle d_{xz}|$, $\langle d_{yz}|$
  * ket: $|d_{xy}\rangle$, $|d_{xz}\rangle$, $|d_{yz}\rangle$
  * wyckoff: `6b@3c`

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

$\boxed{\text{z5}}$ $\mathbb{Q}_{0}^{(c)}(A_{1g},b) = \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{5} + \frac{\sqrt{5}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{5}$

$\boxed{\text{z6}}$ $\mathbb{Q}_{4}^{(c)}(A_{1g}) = \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} - \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{10} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15}$

$\boxed{\text{z8}}$ $\mathbb{G}_{0}^{(c)}(A_{1u}) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{3}$

$\boxed{\text{z17}}$ $\mathbb{G}_{3}^{(c)}(A_{2g}) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(E_g)}{2} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

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

$\boxed{\text{z19}}$ $\mathbb{Q}_{2,1}^{(c)}(E_g,a) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{2}$

$\boxed{\text{z20}}$ $$\mathbb{Q}_{2,2}^{(c)}(E_g,a) = \frac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{2}$$

$\boxed{\text{z21}}$ $$\mathbb{Q}_{2,1}^{(c)}(E_g,b) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$$

$\boxed{\text{z22}}$ $$\mathbb{Q}_{2,2}^{(c)}(E_g,b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{0}^{(b)}(A_{1g})}{2}$$

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

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

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

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

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

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

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

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

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

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

$\boxed{\text{z36}}$ $$\mathbb{Q}_{4,3}^{(c)}(T_{1g}) = \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{6}$$

$\boxed{\text{z46}}$ $$\mathbb{G}_{1,1}^{(c)}(T_{1g}) = -\frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{10} + \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30}$$

$\boxed{\text{z47}}$ $$\mathbb{G}_{1,2}^{(c)}(T_{1g}) = \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} - \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{10} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30}$$

$\boxed{\text{z48}}$ $$\mathbb{G}_{1,3}^{(c)}(T_{1g}) = -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{30} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{15}$$

$\boxed{\text{z49}}$ $$\mathbb{G}_{3,1}^{(c)}(T_{1g}) = \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{20} - \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} - \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{60} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{60} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15}$$

$\boxed{\text{z50}}$ $$\mathbb{G}_{3,2}^{(c)}(T_{1g}) = -\frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{20} + \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{60} + \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_g)}{20} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{60} - \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15}$$

$\boxed{\text{z51}}$ $$\mathbb{G}_{3,3}^{(c)}(T_{1g}) = -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{15} - \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{30} + \frac{\sqrt{30}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{15} + \frac{\sqrt{30}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_g)}{30}$$

$\boxed{\text{z52}}$ $$\mathbb{Q}_{1,1}^{(c)}(T_{1u}, a) = \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}$$

$\boxed{\text{z53}}$ $$\mathbb{Q}_{1,2}^{(c)}(T_{1u}, a) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$\boxed{\text{z54}}$ $$\mathbb{Q}_{1,3}^{(c)}(T_{1u}, a) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$$

$\boxed{\text{z55}}$ $$\mathbb{Q}_{1,1}^{(c)}(T_{1u}, b) = \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6}$$

$\boxed{\text{z56}}$ $$\mathbb{Q}_{1,2}^{(c)}(T_{1u}, b) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$\boxed{\text{z57}}$ $$\mathbb{Q}_{1,3}^{(c)}(T_{1u}, b) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$$

$\boxed{\text{z58}}$ $$\mathbb{Q}_{2,1}^{(c)}(T_{2g}, a) = \frac{\sqrt{3}\mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3}$$

$\boxed{\text{z59}}$ $$\mathbb{Q}_{2,2}^{(c)}(T_{2g}, a) = \frac{\sqrt{3}\mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3}$$

$\boxed{\text{z60}}$ $\mathbb{Q}_{2,3}^{(c)}(T_{2g},a) = \frac{\sqrt{3}\mathbb{Q}_{0}^{(a)}(A_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3}$

$\boxed{\text{z62}}$ $\mathbb{Q}_{2,1}^{(c)}(T_{2g},b) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{0}^{(b)}(A_{1g})}{3}$

$\boxed{\text{z63}}$ $\mathbb{Q}_{2,2}^{(c)}(T_{2g},b) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{0}^{(b)}(A_{1g})}{3}$

$\boxed{\text{z66}}$ $\mathbb{Q}_{2,3}^{(c)}(T_{2g},b) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{0}^{(b)}(A_{1g})}{3}$

$\boxed{\text{z67}}$ $\mathbb{Q}_{2,1}^{(c)}(T_{2g},c) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_{g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{42} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{g})}{42} - \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{g})}{14} - \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(E_{g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14}$

$\boxed{\text{z68}}$ $\mathbb{Q}_{2,2}^{(c)}(T_{2g},c) = \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_{g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{42} + \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(E_{g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{g})}{42} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14}$

$\boxed{\text{z69}}$ $\mathbb{Q}_{2,3}^{(c)}(T_{2g},c) = -\frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(E_{g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} + \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{14} + \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{14} - \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{g})}{21}$

$\boxed{\text{z73}}$ $\mathbb{Q}_{4,1}^{(c)}(T_{2g}) = -\frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(E_{g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{28} - \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{g})}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{g})}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_{g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} + \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21}$

$\boxed{\text{z74}}$ $\mathbb{Q}_{4,2}^{(c)}(T_{2g}) = -\frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(E_{g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{21} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(E_{g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{28} - \frac{\sqrt{14}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{g})}{28} - \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{g})}{28} + \frac{\sqrt{42}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21}$

$\boxed{\text{z75}}$ $\mathbb{Q}_{4,3}^{(c)}(T_{2g}) = \frac{\sqrt{14}\mathbb{Q}_{2,1}^{(a)}(E_{g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{14} + \frac{\sqrt{42}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{21} + \frac{\sqrt{42}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{21} + \frac{\sqrt{14}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{g})}{14}$

$\boxed{\text{z76}}$ $\mathbb{G}_{3,1}^{(c)}(T_{2g}) = \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E_{g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{12} - \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{g})}{12} + \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{g})}{4} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{4}$

$\boxed{\text{z77}}$ $\mathbb{G}_{3,2}^{(c)}(T_{2g}) = \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E_{g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{12} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_{g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{4} - \frac{\sqrt{6}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{g})}{12} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_{2,2}^{(b)}(E_{g})}{4}$

$\boxed{\text{z78}}$ $\mathbb{G}_{3,3}^{(c)}(T_{2g}) = -\frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E_{g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{6} + \frac{\sqrt{6}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_{2,1}^{(b)}(E_{g})}{6}$

$\boxed{\text{z82}}$ $\mathbb{Q}_{3,1}^{(c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6}$

$\boxed{\text{z83}}$ $\mathbb{Q}_{3,2}^{(c)}(T_{2u}) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,3}^{(b)}(T_{2u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$

$\boxed{\text{z84}}$ $\mathbb{Q}_{3,3}^{(c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{M}_{2,2}^{(b)}(T_{2u})}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{M}_{2,1}^{(b)}(T_{2u})}{6}$

$\boxed{\text{z85}}$ $\mathbb{G}_{2,1}^{(c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6}$

$\boxed{\text{z86}}$ $\mathbb{G}_{2,2}^{(c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,3}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$

$\boxed{\text{z87}}$ $\mathbb{G}_{2,3}^{(c)}(T_{2u}) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_{1g})\mathbb{T}_{1,2}^{(b)}(T_{1u})}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_{1g})\mathbb{T}_{1,1}^{(b)}(T_{1u})}{6}$

Atomic SAMB

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

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

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

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

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

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

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

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

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

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

— Cluster SAMB

- Site cluster

** Wyckoff: `1a`

$\boxed{\text{y1}}$ $\mathbb{Q}_{0}^{(s)}(A_{1g}) = [1]$

- Bond cluster

** Wyckoff: `3a@3d`

$\boxed{\text{y2}}$ $$\mathbb{Q}_{0}^{(s)}(A_{1g}) = \left[\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}\right]$$

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

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

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

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

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

** Wyckoff: `6b@3c`

y8 $\mathbb{Q}_{0}^{(s)}(A_{1g}) = \left[\frac{\sqrt{6}}{6},\ \frac{\sqrt{6}}{6},\ \frac{\sqrt{6}}{6},\ \frac{\sqrt{6}}{6},\ \frac{\sqrt{6}}{6},\ \frac{\sqrt{6}}{6}\right]$

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

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

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

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

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

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

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

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

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

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

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

Site and Bond

Table 5: Orbital of each site

#	site	orbital
1	V	$\vert d_{xy}\rangle$, $\vert d_{xz}\rangle$, $\vert d_{yz}\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	V	V	[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 ($\boldsymbol{s}$)	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, $|\boldsymbol{v}|$= 3.8409 (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,-3,4,17,-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, $|\boldsymbol{v}|$= 5.43185 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (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]
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]

continued ...

Table 9

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
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]