

# Model for “SrVO<sub>3</sub>”

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## General Condition

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- Basis type: 1g
- SAMB selection:
  - Type: [Q, G]
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [A<sub>1g</sub>, A<sub>2g</sub>, E<sub>g</sub>, T<sub>1g</sub>, T<sub>2g</sub>, A<sub>1u</sub>, A<sub>2u</sub>, E<sub>u</sub>, T<sub>1u</sub>, T<sub>2u</sub>]
  - 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<sub>1g</sub>, A<sub>2g</sub>, E<sub>g</sub>, T<sub>1g</sub>, T<sub>2g</sub>, A<sub>1u</sub>, A<sub>2u</sub>, E<sub>u</sub>, T<sub>1u</sub>, T<sub>2u</sub>]
  - Spin (s): [0, 1]
- Site-cluster selection:
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [A<sub>1g</sub>, A<sub>2g</sub>, E<sub>g</sub>, T<sub>1g</sub>, T<sub>2g</sub>, A<sub>1u</sub>, A<sub>2u</sub>, E<sub>u</sub>, T<sub>1u</sub>, T<sub>2u</sub>]
- Bond-cluster selection:
  - Type: [Q, G, M, T]
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [A<sub>1g</sub>, A<sub>2g</sub>, E<sub>g</sub>, T<sub>1g</sub>, T<sub>2g</sub>, A<sub>1u</sub>, A<sub>2u</sub>, E<sub>u</sub>, T<sub>1u</sub>, T<sub>2u</sub>]
- Max. neighbor: 10
- Search cell range: (-2, 3), (-2, 3), (-2, 3)
- Toroidal priority: false

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## Group and Unit Cell

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- Group: SG No. 221 O<sub>h</sub><sup>1</sup> Pm $\bar{3}m$  [ cubic ]
- Associated point group: PG No. 221 O<sub>h</sub> 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):  
 $\mathbf{a}_1 = [3.84090, 0.00000, 0.00000]$   
 $\mathbf{a}_2 = [0.00000, 3.84090, 0.00000]$   
 $\mathbf{a}_3 = [0.00000, 0.00000, 3.84090]$

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**Symmetry Operation**


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Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	{1 0}	2	{2 <sub>001</sub>  0}	3	{2 <sub>010</sub>  0}	4	{2 <sub>100</sub>  0}	5	{3 <sub>111</sub> <sup>+</sup>  0}
6	{3 <sub>-11-1</sub> <sup>+</sup>  0}	7	{3 <sub>1-1-1</sub> <sup>+</sup>  0}	8	{3 <sub>-1-11</sub> <sup>+</sup>  0}	9	{3 <sub>111</sub> <sup>-</sup>  0}	10	{3 <sub>1-1-1</sub> <sup>-</sup>  0}
11	{3 <sub>-1-11</sub> <sup>-</sup>  0}	12	{3 <sub>-11-1</sub> <sup>-</sup>  0}	13	{2 <sub>110</sub>  0}	14	{2 <sub>1-10</sub>  0}	15	{4 <sub>001</sub> <sup>-</sup>  0}
16	{4 <sub>001</sub> <sup>+</sup>  0}	17	{4 <sub>-100</sub> <sup>-</sup>  0}	18	{2 <sub>011</sub>  0}	19	{2 <sub>01-1</sub>  0}	20	{4 <sub>100</sub> <sup>+</sup>  0}
21	{4 <sub>010</sub> <sup>+</sup>  0}	22	{2 <sub>101</sub>  0}	23	{4 <sub>010</sub> <sup>-</sup>  0}	24	{2 <sub>-101</sub>  0}	25	{-1 0}
26	{m <sub>001</sub>  0}	27	{m <sub>010</sub>  0}	28	{m <sub>100</sub>  0}	29	{-3 <sub>111</sub> <sup>+</sup>  0}	30	{-3 <sub>-11-1</sub> <sup>+</sup>  0}
31	{-3 <sub>1-1-1</sub> <sup>+</sup>  0}	32	{-3 <sub>-1-11</sub> <sup>+</sup>  0}	33	{-3 <sub>111</sub> <sup>-</sup>  0}	34	{-3 <sub>1-1-1</sub> <sup>-</sup>  0}	35	{-3 <sub>-1-11</sub> <sup>-</sup>  0}
36	{-3 <sub>-11-1</sub> <sup>-</sup>  0}	37	{m <sub>110</sub>  0}	38	{m <sub>1-10</sub>  0}	39	{-4 <sub>001</sub> <sup>-</sup>  0}	40	{-4 <sub>001</sub> <sup>+</sup>  0}
41	{-4 <sub>-100</sub> <sup>-</sup>  0}	42	{m <sub>011</sub>  0}	43	{m <sub>01-1</sub>  0}	44	{-4 <sub>100</sub> <sup>+</sup>  0}	45	{-4 <sub>010</sub> <sup>+</sup>  0}
46	{m <sub>101</sub>  0}	47	{-4 <sub>010</sub> <sup>-</sup>  0}	48	{m <sub>-101</sub>  0}				

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**Harmonics**


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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	$Q, T$	-	-	$\frac{\sqrt{21}(x^4 - 3x^2y^2 - 3x^2z^2 + y^4 - 3y^2z^2 + z^4)}{6}$
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	$\frac{\sqrt{35}xy(x-y)(x+y)}{2}$
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	$\frac{\sqrt{5}yz(6x^2-y^2-z^2)}{2}$
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	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$

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Basis in full matrix

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Table 3: dimension = 3

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

Table 4: Atomic basis (orbital part only)

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

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— SAMB: 87 (all 87) —

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- 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

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

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

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

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

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

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

- V;V\_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

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

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

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

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

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

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

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

$$\boxed{\text{z15}} \quad \mathbb{Q}_{2,2}^{(c)}(E_g, b) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E_g)\mathbb{Q}_0^{(b)}(A_{1g})}{2}$$

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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{z61}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, a) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z64}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, a) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z65}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, a) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

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

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

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

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

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

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

• **V;V\_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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boxed{\text{z58}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, a) = \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,1}^{(b)}(T_{2g})}{3}$$

$$\boxed{\text{z59}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, a) = \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,2}^{(b)}(T_{2g})}{3}$$

$$\boxed{\text{z60}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, a) = \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_{1g})\mathbb{Q}_{2,3}^{(b)}(T_{2g})}{3}$$

$$\boxed{\text{z62}} \quad \mathbb{Q}_{2,1}^{(c)}(T_{2g}, b) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z63}} \quad \mathbb{Q}_{2,2}^{(c)}(T_{2g}, b) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

$$\boxed{\text{z66}} \quad \mathbb{Q}_{2,3}^{(c)}(T_{2g}, b) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_{2g})\mathbb{Q}_0^{(b)}(A_{1g})}{3}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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### — Atomic SAMB —

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

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

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

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

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

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

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

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

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

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

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### — Cluster SAMB —

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- Site cluster

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

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

- Bond cluster

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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— Site and Bond —

Table 5: Orbital of each site

#	site	orbital
1	v	$ d_{xy}\rangle,  d_{xz}\rangle,  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]

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— Site in Unit Cell —

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

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

SL	position ( $s$ )	mapping
1	[ 0.00000, 0.00000, 0.00000]	[1,2,3,4, $\dots$ ,48]

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— Bond in Unit Cell —

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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,  $|v|=3.8409$  (cartesian)

SL	vector ( $v$ )	center ( $c$ )	mapping	head	tail	$R$ (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,  $|v|=5.43185$  (cartesian)

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