

Model for “GaAs”

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General Condition

- Basis type: 1g
- SAMB selection:
 - Type: [Q, G]
 - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
 - Irrep.: [A₁, A₂, E, T₁, T₂]
 - Spin (s): [0, 1]
- Max. neighbor: 10
- Search cell range: (-2, 3), (-2, 3), (-2, 3)
- Toroidal priority: false

Group and Unit Cell

- Group: SG No. 216 T_d^2 $F\bar{4}3m$ [cubic]
- Associated point group: PG No. 216 T_d $\bar{4}3m$ [cubic]
- Unit cell:
 $a = 1.00000, b = 1.00000, c = 1.00000, \alpha = 90.0, \beta = 90.0, \gamma = 90.0$
- Lattice vectors (conventional cell):
 $a_1 = [1.00000, 0.00000, 0.00000]$
 $a_2 = [0.00000, 1.00000, 0.00000]$
 $a_3 = [0.00000, 0.00000, 1.00000]$
- Plus sets:
 $+ [0, 0, 0], + [0, \frac{1}{2}, \frac{1}{2}], + [\frac{1}{2}, 0, \frac{1}{2}], + [\frac{1}{2}, \frac{1}{2}, 0]$

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	{m ₁₋₁₀ 0}	14	{m ₁₁₀ 0}	15	{-4 ₀₀₁ ⁺ 0}
16	{-4 ₀₀₁ ⁻ 0}	17	{m ₀₁₋₁ 0}	18	{-4 ₁₀₀ ⁺ 0}	19	{-4 ₁₀₀ ⁻ 0}	20	{m ₀₁₁ 0}
21	{m ₋₁₀₁ 0}	22	{-4 ₀₁₀ ⁻ 0}	23	{m ₁₀₁ 0}	24	{-4 ₀₁₀ ⁺ 0}		

 — Harmonics —

Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A_1)$	A_1	0	Q, T	-	-	1
2	$\mathbb{Q}_3(A_1)$	A_1	3	Q, T	-	-	$\sqrt{15}xyz$
3	$\mathbb{G}_0(A_2)$	A_2	0	G, M	-	-	1
4	$\mathbb{G}_{2,1}(E)$	E	2	G, M	-	1	$-\frac{\sqrt{3}(x-y)(x+y)}{2}$
5	$\mathbb{G}_{2,2}(E)$					2	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
6	$\mathbb{Q}_{2,1}(E)$	E	2	Q, T	-	1	$-\frac{x^2}{2} - \frac{y^2}{2} + z^2$
7	$\mathbb{Q}_{2,2}(E)$					2	$\frac{\sqrt{3}(x-y)(x+y)}{2}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
8	$\mathbb{G}_{1,1}(T_1)$	T_1	1	G, M	-	1	x
9	$\mathbb{G}_{1,2}(T_1)$					2	y
10	$\mathbb{G}_{1,3}(T_1)$					3	z
11	$\mathbb{G}_{2,1}(T_1)$	T_1	2	G, M	-	1	$\sqrt{3}yz$
12	$\mathbb{G}_{2,2}(T_1)$					2	$\sqrt{3}xz$
13	$\mathbb{G}_{2,3}(T_1)$					3	$\sqrt{3}xy$
14	$\mathbb{Q}_{3,1}(T_1)$	T_1	3	Q, T	-	1	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
15	$\mathbb{Q}_{3,2}(T_1)$					2	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
16	$\mathbb{Q}_{3,3}(T_1)$					3	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
17	$\mathbb{Q}_{1,1}(T_2)$	T_2	1	Q, T	-	1	x
18	$\mathbb{Q}_{1,2}(T_2)$					2	y
19	$\mathbb{Q}_{1,3}(T_2)$					3	z
20	$\mathbb{Q}_{2,1}(T_2)$	T_2	2	Q, T	-	1	$\sqrt{3}yz$
21	$\mathbb{Q}_{2,2}(T_2)$					2	$\sqrt{3}xz$
22	$\mathbb{Q}_{2,3}(T_2)$					3	$\sqrt{3}xy$
23	$\mathbb{Q}_{3,1}(T_2)$	T_2	3	Q, T	-	1	$\frac{x(2x^2-3y^2-3z^2)}{2}$
24	$\mathbb{Q}_{3,2}(T_2)$					2	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
25	$\mathbb{Q}_{3,3}(T_2)$					3	$-\frac{z(3x^2+3y^2-2z^2)}{2}$

— Basis in full matrix —

Table 3: dimension = 6

#	orbital@atom(SL)								
0	$ p_x\rangle @\text{As}(1)$	1	$ p_y\rangle @\text{As}(1)$	2	$ p_z\rangle @\text{As}(1)$	3	$ p_x\rangle @\text{Ga}(1)$	4	$ p_y\rangle @\text{Ga}(1)$
5	$ p_z\rangle @\text{Ga}(1)$								

Table 4: Atomic basis (orbital part only)

orbital	definition
$ p_x\rangle$	x
$ p_y\rangle$	y
$ p_z\rangle$	z

SAMB

21 (all 48) SAMBs

- 'As' site-cluster
 - * bra: $\langle p_x |, \langle p_y |, \langle p_z |$
 - * ket: $|p_x \rangle, |p_y \rangle, |p_z \rangle$
 - * wyckoff: 4c

$$\boxed{\text{z1}} \quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1) \mathbb{Q}_0^{(s)}(A_1)$$

$$\boxed{\text{z6}} \quad \mathbb{Q}_{2,1}^{(c)}(E) = \frac{\sqrt{2} \mathbb{Q}_{2,1}^{(a)}(E) \mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{\text{z7}} \quad \mathbb{Q}_{2,2}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{\text{z28}} \quad \mathbb{Q}_{2,1}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_0^{(s)}(A_1)}{3}$$

$$\boxed{\text{z29}} \quad \mathbb{Q}_{2,2}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_0^{(s)}(A_1)}{3}$$

$$\boxed{\text{z30}} \quad \mathbb{Q}_{2,3}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_0^{(s)}(A_1)}{3}$$

- 'Ga' site-cluster
 - * bra: $\langle p_x |, \langle p_y |, \langle p_z |$
 - * ket: $|p_x \rangle, |p_y \rangle, |p_z \rangle$
 - * wyckoff: 4a

$$\boxed{\text{z2}} \quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(s)}(A_1)$$

$$\boxed{\text{z8}} \quad \mathbb{Q}_{2,1}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{\text{z9}} \quad \mathbb{Q}_{2,2}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{\text{z31}} \quad \mathbb{Q}_{2,1}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_0^{(s)}(A_1)}{3}$$

$$\boxed{\text{z32}} \quad \mathbb{Q}_{2,2}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_0^{(s)}(A_1)}{3}$$

$$\boxed{\text{z33}} \quad \mathbb{Q}_{2,3}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_0^{(s)}(A_1)}{3}$$

- 'As'-'Ga' bond-cluster
 - * bra: $\langle p_x |, \langle p_y |, \langle p_z |$
 - * ket: $|p_x \rangle, |p_y \rangle, |p_z \rangle$
 - * wyckoff: 16a@16e

$$\boxed{\text{z3}} \quad \mathbb{Q}_0^{(c)}(A_1) = \mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_0^{(b)}(A_1)$$

$$\boxed{\text{z4}} \quad \mathbb{Q}_3^{(c)}(A_1) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_{1,3}^{(b)}(T_2)}{3}$$

$$\boxed{\text{z5}} \quad \mathbb{G}_0^{(c)}(A_2) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_1)\mathbb{T}_{1,1}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_1)\mathbb{T}_{1,2}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_1)\mathbb{T}_{1,3}^{(b)}(T_2)}{3}$$

$$\boxed{\text{z10}} \quad \mathbb{Q}_{2,1}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z11}} \quad \mathbb{Q}_{2,2}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z12}} \quad \mathbb{G}_{2,1}^{(c)}(E, a) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{6} + \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{6} - \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_{1,3}^{(b)}(T_2)}{3}$$

$$\boxed{\text{z13}} \quad \mathbb{G}_{2,2}^{(c)}(E, a) = -\frac{\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{2}$$

$$\boxed{\text{z14}} \quad \mathbb{G}_{2,1}^{(c)}(E, b) = -\frac{\mathbb{M}_{1,1}^{(a)}(T_1)\mathbb{T}_{1,1}^{(b)}(T_2)}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(T_1)\mathbb{T}_{1,2}^{(b)}(T_2)}{2}$$

$$\boxed{\text{z15}} \quad \mathbb{G}_{2,2}^{(c)}(E, b) = -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_1)\mathbb{T}_{1,1}^{(b)}(T_2)}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_1)\mathbb{T}_{1,2}^{(b)}(T_2)}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_1)\mathbb{T}_{1,3}^{(b)}(T_2)}{3}$$

$$\boxed{\text{z16}} \quad \mathbb{Q}_{3,1}^{(c)}(T_1) = -\frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_{1,1}^{(b)}(T_2)}{6} - \frac{\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_{1,1}^{(b)}(T_2)}{6} - \frac{\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_{1,3}^{(b)}(T_2)}{3} + \frac{\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{3}$$

$$\boxed{\text{z17}} \quad \mathbb{Q}_{3,2}^{(c)}(T_1) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_{1,2}^{(b)}(T_2)}{6} + \frac{\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_{1,3}^{(b)}(T_2)}{3} - \frac{\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_{1,2}^{(b)}(T_2)}{6} - \frac{\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{3}$$

$$\boxed{\text{z18}} \quad \mathbb{Q}_{3,3}^{(c)}(T_1) = -\frac{\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{3} + \frac{\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_{1,3}^{(b)}(T_2)}{3} + \frac{\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{3}$$

$$\boxed{\text{z19}} \quad \mathbb{G}_{1,1}^{(c)}(T_1) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_1)\mathbb{T}_0^{(b)}(A_1)}{3}$$

$$\boxed{\text{z20}} \quad \mathbb{G}_{1,2}^{(c)}(T_1) = \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_1)\mathbb{T}_0^{(b)}(A_1)}{3}$$

$$\boxed{\text{z21}} \quad \mathbb{G}_{1,3}^{(c)}(T_1) = \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_1)\mathbb{T}_0^{(b)}(A_1)}{3}$$

$$\boxed{\text{z22}} \quad \mathbb{G}_{2,1}^{(c)}(T_1, a) = \frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_{1,1}^{(b)}(T_2)}{6} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_{1,1}^{(b)}(T_2)}{6} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_{1,3}^{(b)}(T_2)}{6} + \frac{\sqrt{2}\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{6}$$

$$\boxed{\text{z23}} \quad \mathbb{G}_{2,2}^{(c)}(T_1, a) = -\frac{\sqrt{6}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_{1,2}^{(b)}(T_2)}{6} + \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_{1,3}^{(b)}(T_2)}{6} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_{1,2}^{(b)}(T_2)}{6} - \frac{\sqrt{2}\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{6}$$

$$\boxed{\text{z24}} \quad \mathbb{G}_{2,3}^{(c)}(T_1, a) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{6} - \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_{1,3}^{(b)}(T_2)}{3} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{6}$$

$$\boxed{\text{z25}} \quad \mathbb{G}_{2,1}^{(c)}(T_1, b) = \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_1)\mathbb{T}_{1,3}^{(b)}(T_2)}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_1)\mathbb{T}_{1,2}^{(b)}(T_2)}{6}$$

$$\boxed{\text{z26}} \quad \mathbb{G}_{2,2}^{(c)}(T_1, b) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_1)\mathbb{T}_{1,3}^{(b)}(T_2)}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_1)\mathbb{T}_{1,1}^{(b)}(T_2)}{6}$$

$$\boxed{\text{z27}} \quad \mathbb{G}_{2,3}^{(c)}(T_1, b) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_1)\mathbb{T}_{1,2}^{(b)}(T_2)}{6} + \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_1)\mathbb{T}_{1,1}^{(b)}(T_2)}{6}$$

$$\boxed{\text{z34}} \quad \mathbb{Q}_{1,1}^{(c)}(T_2, a) = \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,1}^{(b)}(T_2)}{3}$$

$$\boxed{\text{z35}} \quad \mathbb{Q}_{1,2}^{(c)}(T_2, a) = \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,2}^{(b)}(T_2)}{3}$$

$$\boxed{\text{z36}} \quad \mathbb{Q}_{1,3}^{(c)}(T_2, a) = \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,3}^{(b)}(T_2)}{3}$$

$$\boxed{\text{z37}} \quad \mathbb{Q}_{1,1}^{(c)}(T_2, b) = -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_{1,1}^{(b)}(T_2)}{30} + \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_{1,1}^{(b)}(T_2)}{10} + \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_{1,3}^{(b)}(T_2)}{10} + \frac{\sqrt{10}\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{10}$$

$$\boxed{\text{z38}} \quad \mathbb{Q}_{1,2}^{(c)}(T_2, b) = -\frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_{1,2}^{(b)}(T_2)}{30} + \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_{1,3}^{(b)}(T_2)}{10} - \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_{1,2}^{(b)}(T_2)}{10} + \frac{\sqrt{10}\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{10}$$

$$\boxed{\text{z39}} \quad \mathbb{Q}_{1,3}^{(c)}(T_2, b) = \frac{\sqrt{30}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_{1,3}^{(b)}(T_2)}{15} + \frac{\sqrt{10}\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{10} + \frac{\sqrt{10}\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{10}$$

$$\boxed{\text{z40}} \quad \mathbb{Q}_{1,1}^{(c)}(T_2, c) = \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_1)\mathbb{T}_{1,3}^{(b)}(T_2)}{6} - \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_1)\mathbb{T}_{1,2}^{(b)}(T_2)}{6}$$

$$\boxed{\text{z41}} \quad \mathbb{Q}_{1,2}^{(c)}(T_2, c) = -\frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_1)\mathbb{T}_{1,3}^{(b)}(T_2)}{6} + \frac{\sqrt{6}\mathbb{M}_{1,3}^{(a)}(T_1)\mathbb{T}_{1,1}^{(b)}(T_2)}{6}$$

$$\boxed{\text{z42}} \quad \mathbb{Q}_{1,3}^{(c)}(T_2, c) = \frac{\sqrt{6}\mathbb{M}_{1,1}^{(a)}(T_1)\mathbb{T}_{1,2}^{(b)}(T_2)}{6} - \frac{\sqrt{6}\mathbb{M}_{1,2}^{(a)}(T_1)\mathbb{T}_{1,1}^{(b)}(T_2)}{6}$$

$$\boxed{\text{z43}} \quad \mathbb{Q}_{2,1}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_0^{(b)}(A_1)}{3}$$

$$\boxed{\text{z44}} \quad \mathbb{Q}_{2,2}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_0^{(b)}(A_1)}{3}$$

$$\boxed{\text{z45}} \quad \mathbb{Q}_{2,3}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_0^{(b)}(A_1)}{3}$$

$$\boxed{\text{z46}} \quad \mathbb{Q}_{3,1}^{(c)}(T_2) = -\frac{\sqrt{5}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_{1,1}^{(b)}(T_2)}{10} + \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_{1,1}^{(b)}(T_2)}{10} - \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_{1,3}^{(b)}(T_2)}{15} - \frac{\sqrt{15}\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{15}$$

$$\boxed{\text{z47}} \quad \mathbb{Q}_{3,2}^{(c)}(T_2) = -\frac{\sqrt{5}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_{1,2}^{(b)}(T_2)}{10} - \frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_{1,3}^{(b)}(T_2)}{15} - \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_{1,2}^{(b)}(T_2)}{10} - \frac{\sqrt{15}\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{15}$$

$$\boxed{\text{z48}} \quad \mathbb{Q}_{3,3}^{(c)}(T_2) = \frac{\sqrt{5}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_{1,3}^{(b)}(T_2)}{5} - \frac{\sqrt{15}\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{15} - \frac{\sqrt{15}\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{15}$$

— Atomic SAMB —

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

$$\boxed{\text{x1}} \quad \mathbb{Q}_0^{(a)}(A_1) = \begin{bmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$$

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

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

$$\boxed{x4} \quad \mathbb{Q}_{2,1}^{(a)}(T_2) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$$

$$\boxed{x5} \quad \mathbb{Q}_{2,2}^{(a)}(T_2) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{x6} \quad \mathbb{Q}_{2,3}^{(a)}(T_2) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\boxed{x7} \quad \mathbb{M}_{1,1}^{(a)}(T_1) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$$

$$\boxed{x8} \quad \mathbb{M}_{1,2}^{(a)}(T_1) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{2} & 0 & 0 \end{bmatrix}$$

$$\boxed{x9} \quad \mathbb{M}_{1,3}^{(a)}(T_1) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

— Cluster SAMB —

- Site cluster

** Wyckoff: **4c**

$$\boxed{y1} \quad \mathbb{Q}_0^{(s)}(A_1) = [1]$$

** Wyckoff: **4a**

$$\boxed{y2} \quad \mathbb{Q}_0^{(s)}(A_1) = [1]$$

- Bond cluster

** Wyckoff: **16a@16e**

$$\boxed{y3} \quad \mathbb{Q}_0^{(s)}(A_1) = \left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right]$$

$$\boxed{y4} \quad \mathbb{T}_0^{(s)}(A_1) = \left[\frac{i}{2}, \frac{i}{2}, \frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{y5} \quad \mathbb{Q}_{1,1}^{(s)}(T_2) = \left[\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2} \right]$$

$$\boxed{y6} \quad \mathbb{Q}_{1,2}^{(s)}(T_2) = \left[\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{y7} \quad \mathbb{Q}_{1,3}^{(s)}(T_2) = \left[\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2} \right]$$

$$\boxed{y8} \quad \mathbb{T}_{1,1}^{(s)}(T_2) = \left[\frac{i}{2}, -\frac{i}{2}, -\frac{i}{2}, \frac{i}{2} \right]$$

$$\boxed{y9} \quad \mathbb{T}_{1,2}^{(s)}(T_2) = \left[\frac{i}{2}, -\frac{i}{2}, \frac{i}{2}, -\frac{i}{2} \right]$$

$$\boxed{y10} \quad \mathbb{T}_{1,3}^{(s)}(T_2) = \left[\frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, -\frac{i}{2} \right]$$

— Site and Bond —

Table 5: Orbital of each site

#	site	orbital
1	As	$ p_x\rangle, p_y\rangle, p_z\rangle$

2	Ga	$ p_x\rangle, p_y\rangle, p_z\rangle$
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Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	As	Ga	[1]	[p]	[p]

— Site in Unit Cell —

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

Table 7: 'As' (#1) site cluster (4c), -43m

SL	position (s)	mapping
1	[0.25000, 0.25000, 0.25000]	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24]

Table 8: 'Ga' (#2) site cluster (4a), -43m

SL	position (s)	mapping
1	[0.00000, 0.00000, 0.00000]	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24]

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 9: 1-th 'As'-'Ga' [1] (#1) bond cluster (16a@16e), D, $|v|=0.43301$ (cartesian)

SL	vector (v)	center (c)	mapping	head	tail	R (primitive)
1	[0.25000, 0.25000, 0.25000]	[0.12500, 0.12500, 0.12500]	[1,5,9,13,17,21]	(1,1)	(1,1)	[0,0,0]
2	[-0.25000,-0.25000, 0.25000]	[0.87500, 0.87500, 0.12500]	[2,7,12,14,19,24]	(1,4)	(1,1)	[0,0,1]
3	[-0.25000, 0.25000,-0.25000]	[0.87500, 0.12500, 0.87500]	[3,8,10,16,18,23]	(1,3)	(1,1)	[0,1,0]
4	[0.25000,-0.25000,-0.25000]	[0.12500, 0.87500, 0.87500]	[4,6,11,15,20,22]	(1,2)	(1,1)	[1,0,0]