

Model for “GaAs”

Generated on 2026-02-01 11:19:10 by MultiPie 2.0.7

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_1 , A_2 , E , T_1 , T_2]**
 - 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_1 , A_2 , E , T_1 , T_2]**
 - Spin (s): **[0, 1]**
- Site-cluster selection:
 - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
 - Irrep.: **[A_1 , A_2 , E , T_1 , T_2]**
- Bond-cluster selection:
 - Type: **[Q, G, M, T]**
 - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
 - Irrep.: **[A_1 , A_2 , E , T_1 , T_2]**
- 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):
 - $\mathbf{a}_1 = [1.00000, 0.00000, 0.00000]$
 - $\mathbf{a}_2 = [0.00000, 1.00000, 0.00000]$
 - $\mathbf{a}_3 = [0.00000, 0.00000, 1.00000]$

- Plus sets:
 $+ [0, 0, 0], \quad + [0, \frac{1}{2}, \frac{1}{2}], \quad + [\frac{1}{2}, 0, \frac{1}{2}], \quad + [\frac{1}{2}, \frac{1}{2}, 0]$

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 |

continued ...

Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|----|-------------------------|--------|------|--------|--------------|-----------|--|
| 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 | $\frac{\sqrt{3}(x-y)(x+y)}{2}$ |
| 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 | $-\frac{y(3x^2-2y^2+3z^2)}{2}$ |

continued ...

Table 2

| # | symbol | irrep. | rank | X | multiplicity | component | symmetry |
|----|-------------------------|--------|------|---|--------------|-----------|--------------------------------|
| 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) | # | orbital@atom(SL) | # | orbital@atom(SL) | # | orbital@atom(SL) | # | 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 |

48 (all 48) SAMBs

• 'As' site-cluster : **As**

* 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 : **Ga**

* 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 : Ga;As_001_1

* bra: $\langle p_x |, \langle p_y |, \langle p_z |$

* ket: $|p_x\rangle, |p_y\rangle, |p_z\rangle$

* wyckoff: 16a@16e

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Cluster SAMB

- Site cluster

** Wyckoff: 4a

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

** Wyckoff: 4c

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

- Bond cluster

** Wyckoff: 16a016e

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

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

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

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

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

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

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

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

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$ |

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), $\bar{4}3m$

| SL | position (\mathbf{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, $|\mathbf{v}|=0.43301$ (cartesian)

| SL | vector (\mathbf{v}) | center (\mathbf{c}) | mapping | head | tail | \mathbf{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] |