# $Tb_{11}Si_4In_6$ Structure: A6B4C11_tI84_139_hm_dei_eh2n-001

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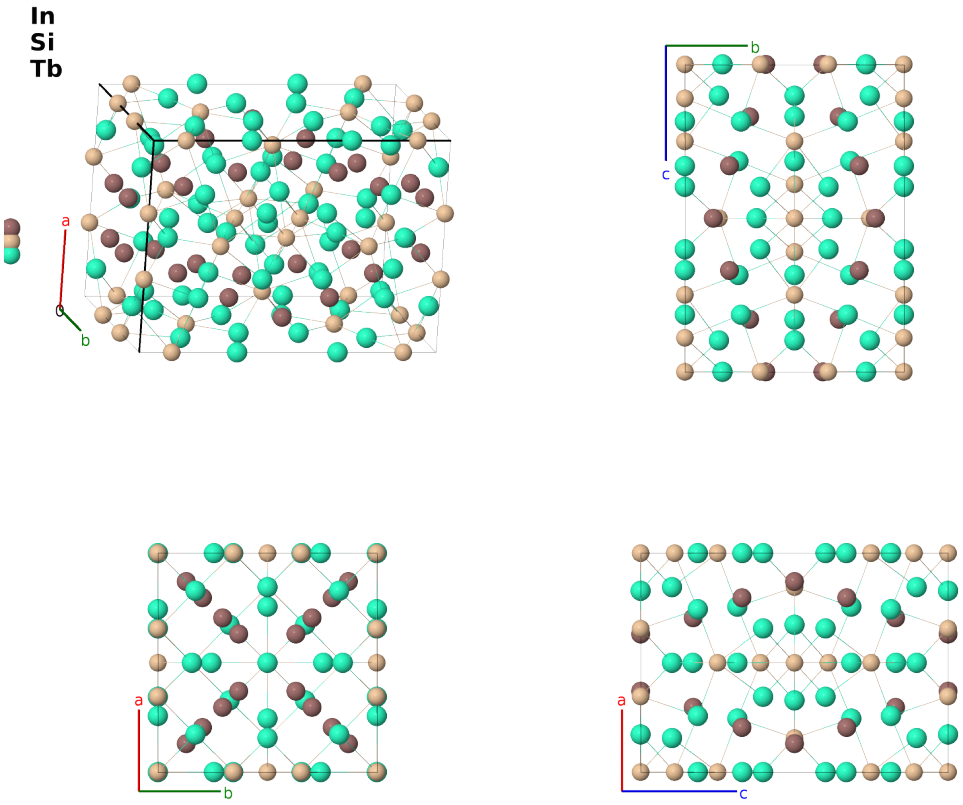
https://aflow.org/prototype-encyclopedia/0KJ3

https://aflow.org/prototype-encyclopedia/A6B4C11_tI84_139_hm_dei_eh2n-001




| | |
|---|---|
| **Prototype** | $In_6Si_4Tb_{11}$ |
| **AFLOW prototype label** | A6B4C11_tI84_139_hm_dei_eh2n-001 |
| **ICSD** | 184236 |
| **CCDC** | 1693480 |
| **Pearson symbol** | tI84 |
| **Space group number** | 139 |
| **Space group symbol** | $I4/mmm$ |
| **AFLOW prototype command** | `aflow --proto=A6B4C11_tI84_139_hm_dei_eh2n-001 --params=`$a, c/a, z_2, z_3, x_4, x_5, x_6, x_7, z_7, y_8, z_8, y_9, z_9$ |

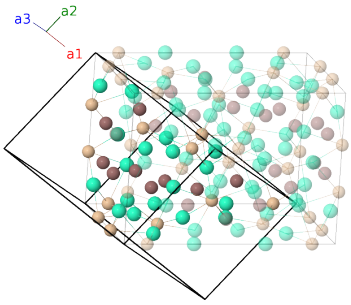
**Other compounds with this structure**

$Dy_{11}Ge_4In_6$, $Dy_{11}Si_4In_6$, $Er_{11}Ge_4In_6$, $Er_{11}Si_4In_6$, $Gd_{11}Ge_4In_6$, $Gd_{11}Si_4In_6$, $Ho_{11}Ge_4In_6$, $Ho_{11}Si_4In_6$, $La_{11}Ge_4In_6$, $Tb_{11}Ge_4In_6$, $Y_{11}Ge_4In_6$, $Y_{11}Si_4In_6$

- This is a tenary form of $Ho_{11}Ge_{10}$. The ICSD lists all these compounds using the $Ho_{11}Ge_{10}$ prototype. $Tb_{11}Si_4In_6$ is the first ICSD entry in the reference, so we use it as the ternary prototype.
- $Sc_{11}Al_2Ge_8$ is a second ternary form of $Ho_{11}Ge_{10}$.
- The AFLOW standard labeling algorithm shifts the origin by (0.5 a, 0.5 b, 0), moving the Si III atom from the published (8j) Wyckoff position to (8i).

**Body-centered Tetragonal primitive vectors**

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$




**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4d) | Si I |
| $\mathbf{B_2}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4d) | Si I |
| $\mathbf{B_3}$ | = | $z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$ | = | $cz_2\,\hat{\mathbf{z}}$ | (4e) | Si II |
| $\mathbf{B_4}$ | = | $-z_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_2$ | = | $-cz_2\,\hat{\mathbf{z}}$ | (4e) | Si II |
| $\mathbf{B_5}$ | = | $z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$ | = | $cz_3\,\hat{\mathbf{z}}$ | (4e) | Tb I |
| $\mathbf{B_6}$ | = | $-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$ | = | $-cz_3\,\hat{\mathbf{z}}$ | (4e) | Tb I |
| $\mathbf{B_7}$ | = | $x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + 2x_4\,\mathbf{a}_3$ | = | $ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$ | (8h) | In I |
| $\mathbf{B_8}$ | = | $-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - 2x_4\,\mathbf{a}_3$ | = | $-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$ | (8h) | In I |
| $\mathbf{B_9}$ | = | $x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$ | = | $-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$ | (8h) | In I |
| $\mathbf{B_{10}}$ | = | $-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$ | = | $ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$ | (8h) | In I |
| $\mathbf{B_{11}}$ | = | $x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + 2x_5\,\mathbf{a}_3$ | = | $ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}}$ | (8h) | Tb II |
| $\mathbf{B_{12}}$ | = | $-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - 2x_5\,\mathbf{a}_3$ | = | $-ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}}$ | (8h) | Tb II |
| $\mathbf{B_{13}}$ | = | $x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2$ | = | $-ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}}$ | (8h) | Tb II |
| $\mathbf{B_{14}}$ | = | $-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2$ | = | $ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}}$ | (8h) | Tb II |
| $\mathbf{B_{15}}$ | = | $x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$ | = | $ax_6\,\hat{\mathbf{x}}$ | (8i) | Si III |
| $\mathbf{B_{16}}$ | = | $-x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$ | = | $-ax_6\,\hat{\mathbf{x}}$ | (8i) | Si III |
| $\mathbf{B_{17}}$ | = | $x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_3$ | = | $ax_6\,\hat{\mathbf{y}}$ | (8i) | Si III |
| $\mathbf{B_{18}}$ | = | $-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_3$ | = | $-ax_6\,\hat{\mathbf{y}}$ | (8i) | Si III |

$$\mathbf{B_{19}} = (x_7 + z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + 2x_7\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad \text{(16m)} \quad \text{In II}$$

$$\mathbf{B_{20}} = -(x_7 - z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - 2x_7\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad \text{(16m)} \quad \text{In II}$$

$$\mathbf{B_{21}} = (x_7 + z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 = -ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad \text{(16m)} \quad \text{In II}$$

$$\mathbf{B_{22}} = -(x_7 - z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 = ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad \text{(16m)} \quad \text{In II}$$

$$\mathbf{B_{23}} = (x_7 - z_7)\,\mathbf{a}_1 - (x_7 + z_7)\,\mathbf{a}_2 = -ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad \text{(16m)} \quad \text{In II}$$

$$\mathbf{B_{24}} = -(x_7 + z_7)\,\mathbf{a}_1 + (x_7 - z_7)\,\mathbf{a}_2 = ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad \text{(16m)} \quad \text{In II}$$

$$\mathbf{B_{25}} = (x_7 - z_7)\,\mathbf{a}_1 + (x_7 - z_7)\,\mathbf{a}_2 + 2x_7\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad \text{(16m)} \quad \text{In II}$$

$$\mathbf{B_{26}} = -(x_7 + z_7)\,\mathbf{a}_1 - (x_7 + z_7)\,\mathbf{a}_2 - 2x_7\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad \text{(16m)} \quad \text{In II}$$

$$\mathbf{B_{27}} = (y_8 + z_8)\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + y_8\,\mathbf{a}_3 = ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad \text{(16n)} \quad \text{Tb III}$$

$$\mathbf{B_{28}} = -(y_8 - z_8)\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 - y_8\,\mathbf{a}_3 = -ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad \text{(16n)} \quad \text{Tb III}$$

$$\mathbf{B_{29}} = z_8\,\mathbf{a}_1 - (y_8 - z_8)\,\mathbf{a}_2 - y_8\,\mathbf{a}_3 = -ay_8\,\hat{\mathbf{x}} + cz_8\,\hat{\mathbf{z}} \quad \text{(16n)} \quad \text{Tb III}$$

$$\mathbf{B_{30}} = z_8\,\mathbf{a}_1 + (y_8 + z_8)\,\mathbf{a}_2 + y_8\,\mathbf{a}_3 = ay_8\,\hat{\mathbf{x}} + cz_8\,\hat{\mathbf{z}} \quad \text{(16n)} \quad \text{Tb III}$$

$$\mathbf{B_{31}} = (y_8 - z_8)\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 + y_8\,\mathbf{a}_3 = ay_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad \text{(16n)} \quad \text{Tb III}$$

$$\mathbf{B_{32}} = -(y_8 + z_8)\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 - y_8\,\mathbf{a}_3 = -ay_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad \text{(16n)} \quad \text{Tb III}$$

$$\mathbf{B_{33}} = -z_8\,\mathbf{a}_1 + (y_8 - z_8)\,\mathbf{a}_2 + y_8\,\mathbf{a}_3 = ay_8\,\hat{\mathbf{x}} - cz_8\,\hat{\mathbf{z}} \quad \text{(16n)} \quad \text{Tb III}$$

$$\mathbf{B_{34}} = -z_8\,\mathbf{a}_1 - (y_8 + z_8)\,\mathbf{a}_2 - y_8\,\mathbf{a}_3 = -ay_8\,\hat{\mathbf{x}} - cz_8\,\hat{\mathbf{z}} \quad \text{(16n)} \quad \text{Tb III}$$

$$\mathbf{B_{35}} = (y_9 + z_9)\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 + y_9\,\mathbf{a}_3 = ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad \text{(16n)} \quad \text{Tb IV}$$

$$\mathbf{B_{36}} = -(y_9 - z_9)\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 - y_9\,\mathbf{a}_3 = -ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad \text{(16n)} \quad \text{Tb IV}$$

$$\mathbf{B_{37}} = z_9\,\mathbf{a}_1 - (y_9 - z_9)\,\mathbf{a}_2 - y_9\,\mathbf{a}_3 = -ay_9\,\hat{\mathbf{x}} + cz_9\,\hat{\mathbf{z}} \quad \text{(16n)} \quad \text{Tb IV}$$

$$\mathbf{B_{38}} = z_9\,\mathbf{a}_1 + (y_9 + z_9)\,\mathbf{a}_2 + y_9\,\mathbf{a}_3 = ay_9\,\hat{\mathbf{x}} + cz_9\,\hat{\mathbf{z}} \quad \text{(16n)} \quad \text{Tb IV}$$

$$\mathbf{B_{39}} = (y_9 - z_9)\,\mathbf{a}_1 - z_9\,\mathbf{a}_2 + y_9\,\mathbf{a}_3 = ay_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \quad \text{(16n)} \quad \text{Tb IV}$$

$$\mathbf{B_{40}} = -(y_9 + z_9)\,\mathbf{a}_1 - z_9\,\mathbf{a}_2 - y_9\,\mathbf{a}_3 = -ay_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \quad \text{(16n)} \quad \text{Tb IV}$$

$$\mathbf{B_{41}} = -z_9\,\mathbf{a}_1 + (y_9 - z_9)\,\mathbf{a}_2 + y_9\,\mathbf{a}_3 = ay_9\,\hat{\mathbf{x}} - cz_9\,\hat{\mathbf{z}} \quad \text{(16n)} \quad \text{Tb IV}$$

$$\mathbf{B_{42}} = -z_9\,\mathbf{a}_1 - (y_9 + z_9)\,\mathbf{a}_2 - y_9\,\mathbf{a}_3 = -ay_9\,\hat{\mathbf{x}} - cz_9\,\hat{\mathbf{z}} \quad \text{(16n)} \quad \text{Tb IV}$$

## References


[1] Y. Tyvanchuk, R. Duraj, T. Jaworska-Gołab, S. Baran, Y. M. Kalychak, J. Przewoźnik, and A. Szytuła, *Structural chemistry and magnetic properties of $R_{11}M_4In_6$ (R = Gd, Tb, Dy, Ho, Er, Y; M = Si, Ge) compounds*, Intermetallics **25**, 18–26 (2012), doi:10.1016/j.intermet.2012.02.005.


## Found in


[1] *Inorganic Crystal Structure Database*. Entry 184236 (Tb11Si4In6).


## First cited in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