# TiFeSi Structure: ABC_oI36_46_ac_bc_3b-001

This structure originally had the label `ABC_oI36_46_ac_bc_3b`. Calls to that address will be redirected here.

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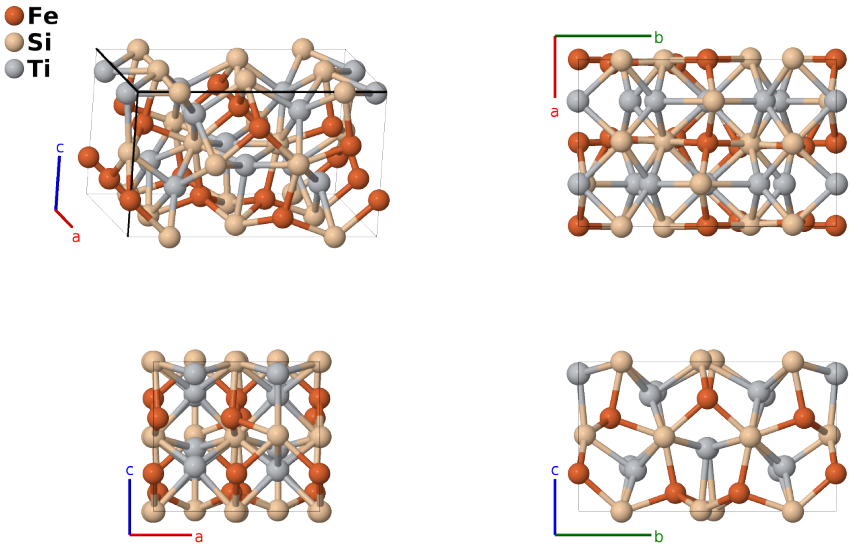
https://aflow.org/p/7FJR

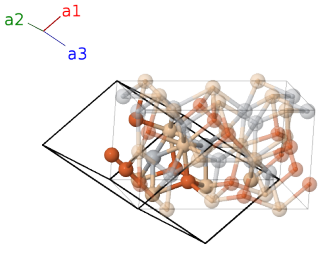
https://aflow.org/p/ABC_oI36_46_ac_bc_3b-001




| | |
|---|---|
| **Prototype** | FeSiTi |
| **AFLOW prototype label** | ABC_oI36_46_ac_bc_3b-001 |
| **ICSD** | 41157 |
| **Pearson symbol** | oI36 |
| **Space group number** | 46 |
| **Space group symbol** | $Ima2$ |
| **AFLOW prototype command** | `aflow --proto=ABC_oI36_46_ac_bc_3b-001 --params=`$a, b/a, c/a, z_1, y_2, z_2, y_3, z_3, y_4, z_4, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$ |

**Body-centered Orthorhombic primitive vectors**

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



**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$ | = | $cz_1\,\hat{\mathbf{z}}$ | (4a) | Fe I |
| $\mathbf{B_2}$ | = | $z_1\,\mathbf{a}_1 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + cz_1\,\hat{\mathbf{z}}$ | (4a) | Fe I |
| $\mathbf{B_3}$ | = | $(y_2 + z_2)\,\mathbf{a}_1 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (4b) | Si I |
| $\mathbf{B_4}$ | = | $-(y_2 - z_2)\,\mathbf{a}_1 + \left(z_2 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (4b) | Si I |
| $\mathbf{B_5}$ | = | $(y_3 + z_3)\,\mathbf{a}_1 + \left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (4b) | Ti I |
| $\mathbf{B_6}$ | = | $-(y_3 - z_3)\,\mathbf{a}_1 + \left(z_3 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(y_3 - \frac{3}{4}\right)\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (4b) | Ti I |
| $\mathbf{B_7}$ | = | $(y_4 + z_4)\,\mathbf{a}_1 + \left(z_4 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_4 + \frac{1}{4}\right)\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (4b) | Ti II |
| $\mathbf{B_8}$ | = | $-(y_4 - z_4)\,\mathbf{a}_1 + \left(z_4 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(y_4 - \frac{3}{4}\right)\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (4b) | Ti II |
| $\mathbf{B_9}$ | = | $(y_5 + z_5)\,\mathbf{a}_1 + \left(z_5 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_5 + \frac{1}{4}\right)\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$ | (4b) | Ti III |
| $\mathbf{B_{10}}$ | = | $-(y_5 - z_5)\,\mathbf{a}_1 + \left(z_5 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(y_5 - \frac{3}{4}\right)\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$ | (4b) | Ti III |
| $\mathbf{B_{11}}$ | = | $(y_6 + z_6)\,\mathbf{a}_1 + (x_6 + z_6)\,\mathbf{a}_2 + (x_6 + y_6)\,\mathbf{a}_3$ | = | $ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8c) | Fe II |
| $\mathbf{B_{12}}$ | = | $-(y_6 - z_6)\,\mathbf{a}_1 - (x_6 - z_6)\,\mathbf{a}_2 - (x_6 + y_6)\,\mathbf{a}_3$ | = | $-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8c) | Fe II |
| $\mathbf{B_{13}}$ | = | $-(y_6 - z_6)\,\mathbf{a}_1 + \left(x_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_6 - y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8c) | Fe II |
| $\mathbf{B_{14}}$ | = | $(y_6 + z_6)\,\mathbf{a}_1 + \left(-x_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_6 + y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8c) | Fe II |
| $\mathbf{B_{15}}$ | = | $(y_7 + z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + (x_7 + y_7)\,\mathbf{a}_3$ | = | $ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (8c) | Si II |
| $\mathbf{B_{16}}$ | = | $-(y_7 - z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - (x_7 + y_7)\,\mathbf{a}_3$ | = | $-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (8c) | Si II |
| $\mathbf{B_{17}}$ | = | $-(y_7 - z_7)\,\mathbf{a}_1 + \left(x_7 + z_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_7 - y_7 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $a\left(x_7 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (8c) | Si II |
| $\mathbf{B_{18}}$ | = | $(y_7 + z_7)\,\mathbf{a}_1 + \left(-x_7 + z_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_7 + y_7 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (8c) | Si II |

**References**


[1] W. Jeitschko, *The Crystal Structure of TiFeSi and Related Compounds*, Acta Crystallogr. Sect. B **26**, 815–822 (1970), doi:10.1107/S0567740870003163.

**Found in**

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.