# $ZrFe_4Si_2$ Structure: A4B2C_tP14_136_i_f_a-001

This structure previously used the label(s) `A4B2C_tP14_136_i_g_b`. Calls to these addresses will be redirected here.

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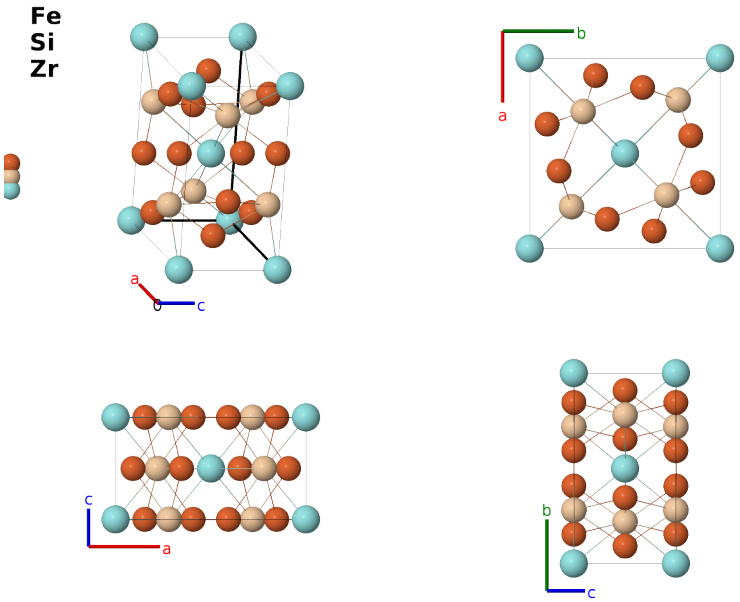
https://aflow.org/prototype-encyclopedia/U6YK

https://aflow.org/prototype-encyclopedia/A4B2C_tP14_136_i_f_a-001




| | |
|---|---|
| **Prototype** | $Fe_4Si_2Zr$ |
| **AFLOW prototype label** | A4B2C_tP14_136_i_f_a-001 |
| **ICSD** | 87172 |
| **CCDC** | 1646993 |
| **Pearson symbol** | tP14 |
| **Space group number** | 136 |
| **Space group symbol** | $P4_2/mnm$ |
| **AFLOW prototype command** | `aflow --proto=A4B2C_tP14_136_i_f_a-001 --params=`$a, c/a, x_2, x_3, y_3$ |

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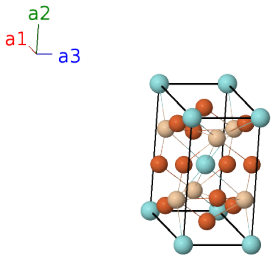
**Other compounds with this structure**

$BaCd_4Pt_2$, $DyFe_4Ge_2$, $DyNi_4As_2$, $ErFe_4Ge_2$, $ErNi_4P_2$, $GdNi_4As_2$, $GdRe_4Si_2$, $HoFe_4Ge_2$, $LuFe_4Ge_2$, $LuNi_4As_2$, $LuRe_4Si_2$, $ScFe_4P_2$, $ScFe_4Si_2$, $ScNi_4As_2$, $SmRe_4Si_2$, $SrCd_4Pt_2$, $TbRe_4Si_2$, $TmFe_4Ge_2$, $TmRe_4Si_2$, $UMn_4P_2$, $YFe_4Ge_2$, $YNi_4As_2$, $YNi_4P_2$, $YRe_4Si_2$, $YbNi_4P_2$, $ZrFe_4P_2$, $ZrNi_4As_2$

## Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$




## Basis vectors

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (2a) | Zr I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (2a) | Zr I |
| $\mathbf{B_3}$ | = | $x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$ | = | $ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$ | (4f) | Si I |
| $\mathbf{B_4}$ | = | $-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$ | = | $-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$ | (4f) | Si I |
| $\mathbf{B_5}$ | = | $-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4f) | Si I |
| $\mathbf{B_6}$ | = | $\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4f) | Si I |
| $\mathbf{B_7}$ | = | $x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2$ | = | $ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}}$ | (8i) | Fe I |
| $\mathbf{B_8}$ | = | $-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2$ | = | $-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}}$ | (8i) | Fe I |
| $\mathbf{B_9}$ | = | $-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (8i) | Fe I |
| $\mathbf{B_{10}}$ | = | $\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (8i) | Fe I |
| $\mathbf{B_{11}}$ | = | $-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (8i) | Fe I |
| $\mathbf{B_{12}}$ | = | $\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (8i) | Fe I |
| $\mathbf{B_{13}}$ | = | $y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$ | = | $ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$ | (8i) | Fe I |
| $\mathbf{B_{14}}$ | = | $-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$ | = | $-ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$ | (8i) | Fe I |

## References


[1] Y. P. Yarmolyuk, L. A. Lysenko, and E. I. Gladyshevsky, *Crystal Structure of $ZrFe_4Si_2$ – A New Structure Type of Ternary Silicides*, Dopov. Akad. Nauk Ukr. RSR, Ser. A **37**, 281–284 (1975). In Russian.


## Found in


[1] P. Schobinger-Papamantellos, J. Rodrıguez-Carvajal, G. André, N. P. Duong, K. H. J. Buschow, and P. Tolédano, *Simultaneous structural and magnetic transitions in $YFe_4Ge_2$ studied by neutron diffraction and magnetic measurements*, J. Magn. Magn. Mater. **236**, 14–27 (2001), doi:10.1016/S0304-8853(01)00442-5.


## First cited in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