

Pseudobrookite (Fe_2TiO_5 , $E4_1$) Structure: A2B5C_oC32_63_f_c2f_c-001

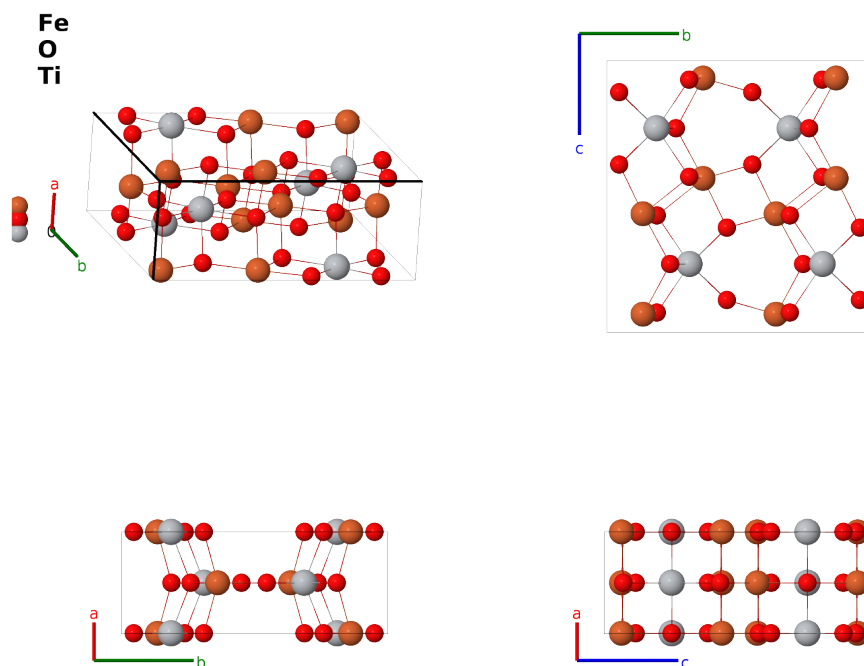
This structure previously used the label(s) **A2B5C_oC32_63_f_c2f_c**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/NJWX>

https://aflow.org/prototype-encyclopedia/A2B5C_oC32_63_f_c2f_c-001



Prototype	$\text{Fe}_2\text{O}_5\text{Ti}$
AFLOW prototype label	A2B5C_oC32_63_f_c2f_c-001
<i>Strukturbericht</i> designation	$E4_1$
Mineral name	pseudobrookite
ICSD	88380
CCDC	1648127
Pearson symbol	oC32
Space group number	63
Space group symbol	$Cmcm$

AFLOW prototype command `aflow --proto=A2B5C_oC32_63_f_c2f_c-001`
 `--params=a, b/a, c/a, y1, y2, y3, z3, y4, z4, y5, z5`

Other compounds with this structure

$\text{Fe}_{1+x}\text{Ti}_{2-x}\text{O}_5$, Ti_2MgO_5 , V_3O_5 (anosovite)

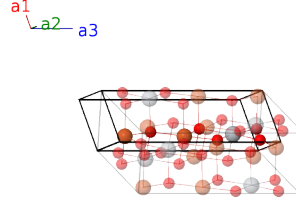
- We use the $x = 1$ data from (Guo, 1999). They find that the site we have labeled Ti I actually has the composition $\text{Fe}_{0.722}\text{Ti}_{0.278}$, while the Fe I site has the composition $\text{Fe}_{0.640}\text{Ti}_{0.360}$, so that the total metallic composition is Fe_2Ti .

Base-centered Orthorhombic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Ti I
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Ti I
$\mathbf{B}_5$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8f)	Fe I
$\mathbf{B}_6$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	Fe I
$\mathbf{B}_7$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	Fe I
$\mathbf{B}_8$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8f)	Fe I
$\mathbf{B}_9$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_{10}$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_{11}$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_{12}$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_{13}$	$= -y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_{14}$	$= y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-by_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_{15}$	$= -y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$by_5 \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B}_{16}$	$= y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8f)	O III

References

- [1] W. Q. Guo, S. Malus, D. H. Ryan, and Z. Altounian, *Crystal structure and cation distributions in the FeTi_2O_5 - Fe_2TiO_5 solid solution series*, J. Phys.: Condens. Matter **11**, 6337–6346 (1999).

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