

Tetrataenite (FeNi) Structure:

AB_mP4_6_2a_2b-001

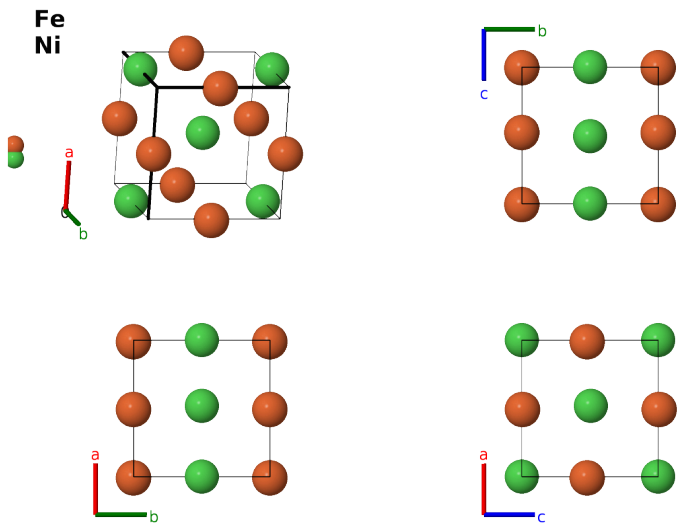
This structure previously used the label(s) **AB_mP4_6_2b_2a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/X3MC>

https://aflow.org/prototype-encyclopedia/AB_mP4_6_2a_2b-001

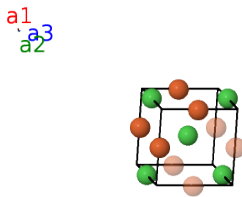


Prototype	FeNi
AFLOW prototype label	AB_mP4_6_2a_2b-001
Mineral name	tetrataenite
ICSD	56386
CCDC	1620633
Pearson symbol	mP4
Space group number	6
Space group symbol	Pm
AFLOW prototype command	<code>aflow --proto=AB_mP4_6_2a_2b-001</code> <code>--params=a,b/a,c/a,β,x_1,z_1,x_2,z_2,x_3,z_3,x_4,z_4</code>

- In the original the site occupations are mixed with Ni majority (0.85) on sites (1a) and Fe majority on (1b).

Simple Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(1a)	Fe I
$\mathbf{B}_2$	$= x_2 \mathbf{a}_1 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(1a)	Fe II
$\mathbf{B}_3$	$= x_3 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(1b)	Ni I
$\mathbf{B}_4$	$= x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(1b)	Ni II

References

- [1] T. Tagai and H. Takeda, *Superstructure of tetrataenite from the Saint Severin meteorite*, Z. für Kristallogr. **210**, 14–18 (1995), doi:10.1524/zkri.1995.210.1.14.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

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