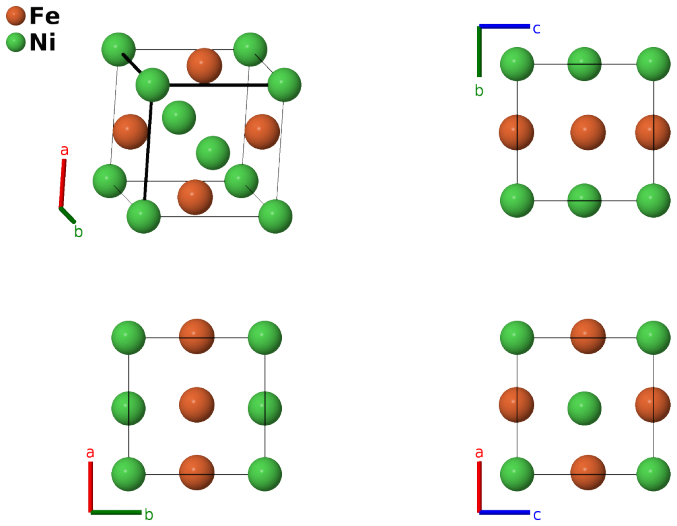
Tetrataenite (FeNi) Structure: AB_mP4_6_2a_2b-001

This structure originally had the label `AB_mP4_6_2b_2a`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

https://aflow.org/p/X3MC

https://aflow.org/p/AB_mP4_6_2a_2b-001

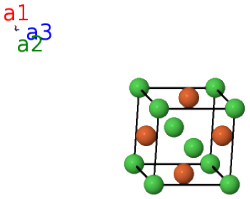


Prototype	FeNi
AFLOW prototype label	AB_mP4_6_2a_2b-001
Mineral name	tetrataenite
ICSD	56386
Pearson symbol	mP4
Space group number	6
Space group symbol	Pm
AFLOW prototype command	`aflow --proto=AB_mP4_6_2a_2b-001 --params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4$

- 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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



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).