

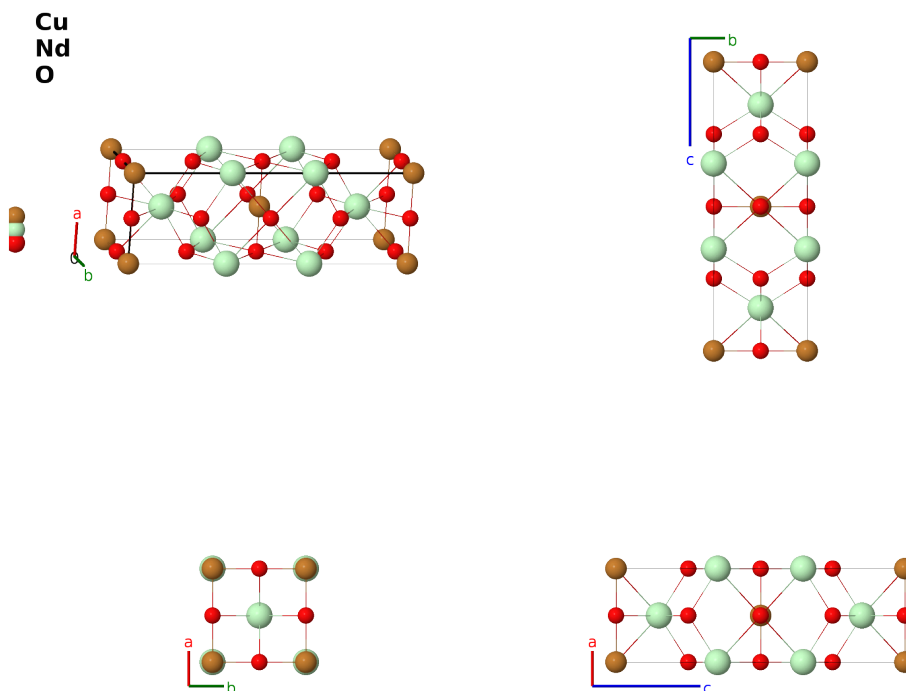
(T') Nd₂CuO₄ Structure: AB2C4_tI14_139_a_e_cd-003

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<https://aflow.org/prototype-encyclopedia/1V8W>

https://aflow.org/prototype-encyclopedia/AB2C4_tI14_139_a_e_cd-003



Prototype	CuNd ₂ O ₄
AFLOW prototype label	AB2C4_tI14_139_a_e_cd-003
ICSD	69886
CCDC	1631723
Pearson symbol	tI14
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	<code>aflow --proto=AB2C4_tI14_139_a_e_cd-003 --params=a, c/a, z₄</code>

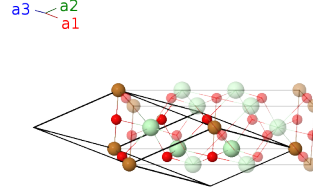
Other compounds with this structure

Eu₂CuO₄, Gd₂CuO₄, La₂CuO₄, Pr₂CuO₄, Sm₂CuO₄

- This is often referred to as the ‘T’- phase of the RE₂CuO₄ compounds.
 - Lattice constants were determined at 80 mK. The value of z_4 for the neodymium atom was determined at 0.5K.
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Body-centered Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) Cu I
$\mathbf{B}_2$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{y}}$	(4c) O I
$\mathbf{B}_3$	=	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}}$	(4c) O I
$\mathbf{B}_4$	=	$\frac{3}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(4d) O II
$\mathbf{B}_5$	=	$\frac{1}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}c\hat{\mathbf{z}}$	(4d) O II
$\mathbf{B}_6$	=	$z_4\mathbf{a}_1 + z_4\mathbf{a}_2$	=	$cz_4\hat{\mathbf{z}}$	(4e) Nd I
$\mathbf{B}_7$	=	$-z_4\mathbf{a}_1 - z_4\mathbf{a}_2$	=	$-cz_4\hat{\mathbf{z}}$	(4e) Nd I

References

- [1] T. Chattopadhyay, P. J. Brown, and U. Kübler, *Crystal and magnetic structure of Nd₂CuO₄ at millikelvin temperatures*, Physica C **177**, 294–296 (1991), doi:10.1016/0921-4534(91)90482-E.

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