(T') Nd_2CuO_4 Structure: AB2C4_tI14_139_a_e_cd-003

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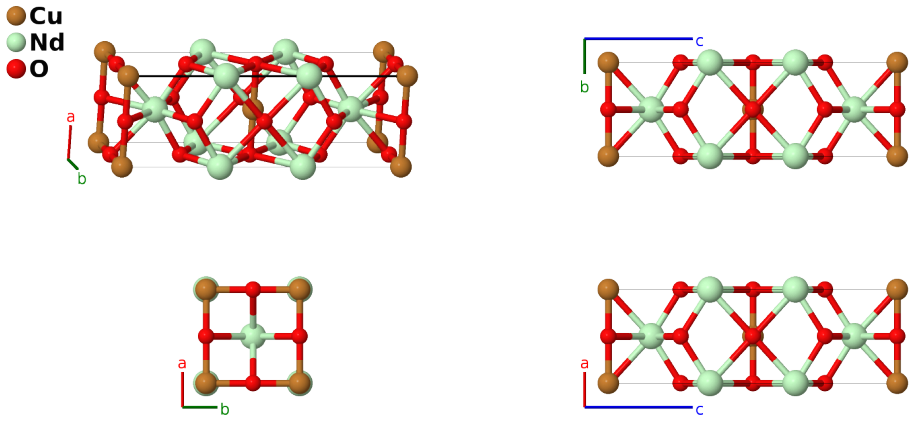


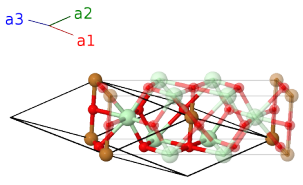
Prototype	$CuNd_2O_4$
AFLOW prototype label	AB2C4_tI14_139_a_e_cd-003
ICSD	69886
Pearson symbol	tI14
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=AB2C4_tI14_139_a_e_cd-003 --params=`$a, c/a, z_4$

Other compounds with this structure
Eu_2CuO_4, Gd_2CuO_4, La_2CuO_4, Pr_2CuO_4, Sm_2CuO_4

- This is often referred to as the 'T'-' phase of the RE_2CuO_4 compounds.
- Lattice constants were determined at 80 mK. The value of z_4 for the neodymium atom was determined at 0.5K.

Body-centered Tetragonal primitive vectors

$$\mathbf{a_1} = -\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - \frac{1}{2}c\,\hat{\mathbf{z}}$$



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 Nd_2CuO_4 at millikelvin temperatures*, Physica C **177**, 294–296 (1991), doi:10.1016/0921-4534(91)90482-E.