$LuNi_2B_2C$ Structure: A2BCD2_tI12_139_e_a_b_d-001

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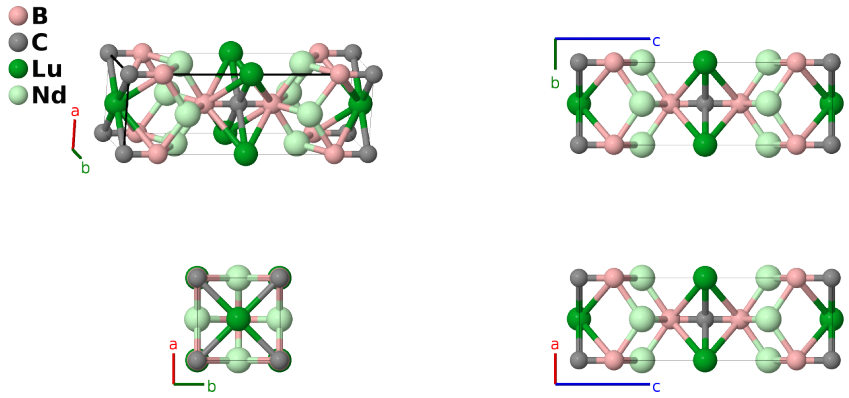
https://aflow.org/p/4LX6

https://aflow.org/p/A2BCD2_tI12_139_e_a_b_d-001

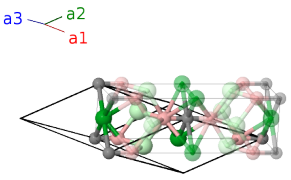


Prototype	B_2CLuNi_2
AFLOW prototype label	A2BCD2_tI12_139_e_a_b_d-001
ICSD	75609
Pearson symbol	tI12
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A2BCD2_tI12_139_e_a_b_d-001 --params=`$a, c/a, z_4$

Other compounds with this structure
GdN_2B_2C, $LaIr_2B_2C$, LaN_2B_2C, $LaPt_2B_2C$, $LaRh_2B_2C$

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)	C I

$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Lu I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Nd I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Nd I
$\mathbf{B_5}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	B I
$\mathbf{B_6}$	=	$-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	B I

References

[1] T. Siegrist, R. J. Cava, J. J. Krajewski, and W. F. P. Jr., *Crystal chemistry of the series LnT_2B_2C (Ln = rare earth, T = transition element)*, J. Alloys Compd. **216**, 135–139 (1994), doi:10.1016/0925-8388(94)91055-3.

Found in

[1] M. W. Pohlkamp and W. Jeitschko, *Preparation, Properties, and Crystal Structure of Quaternary Silicide Carbides RCr_2Si_2C (R = Y, La-Nd, Sm, Gd-Ho)*, Z. Naturforsch. B **56**, 1143–1148 (2001), doi:10.1515/znb-2001-1108.