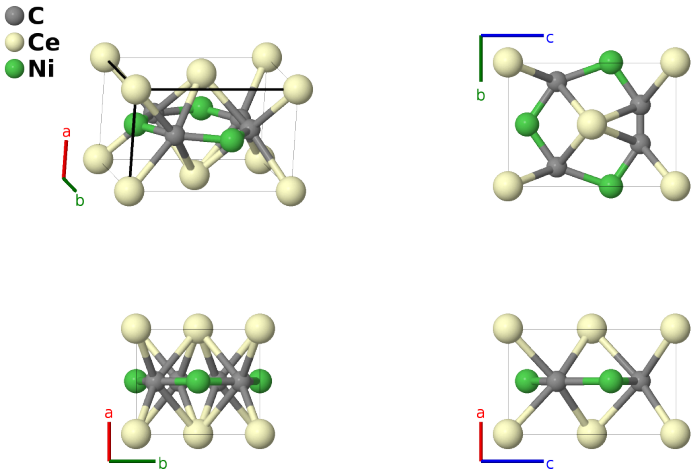
C_2CeNi Structure: A2BC_oC8_38_d_b_a-001

This structure originally had the label `A2BC_oC8_38_e_a_b`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/37DH

https://aflow.org/p/A2BC_oC8_38_d_b_a-001



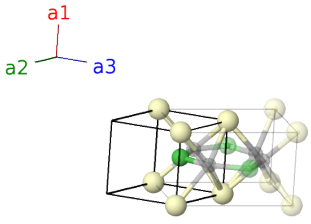
Prototype	C_2CeNi
AFLOW prototype label	A2BC_oC8_38_d_b_a-001
ICSD	20397
Pearson symbol	oC8
Space group number	38
Space group symbol	$Amm2$
AFLOW prototype command	`aflow --proto=A2BC_oC8_38_d_b_a-001 --params=`$a, b/a, c/a, z_1, z_2, y_3, z_3$

Other compounds with this structure

C_2CoDy, C_2CoPu, C_2CoSm, C_2CoTh, C_2ErFe, C_2FeGd, C_2FeSm, C_2NiLa, C_2NiNd, C_2NiPa, C_2NiPr, C_2NiPu, C_2NiSm, C_2NiYb, C_2PrRh

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-z_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Ni I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_2\,\hat{\mathbf{z}}$	(2b)	Ce I
$\mathbf{B_3}$	=	$(y_3 - z_3)\,\mathbf{a}_2 + (y_3 + z_3)\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4d)	C I
$\mathbf{B_4}$	=	$-(y_3 + z_3)\,\mathbf{a}_2 - (y_3 - z_3)\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4d)	C I

References

[1] O. I. Bodak and E. P. Marusin, *The Crystal Structure of $RNiC_2$ Compounds (R=Ce,La,Pr)*, Dopovidia Akademii Nauk Ukrains'koi RSR, Seriya A: Fiziko$_M atematichni Ta Tekhnichni Nauki$**41**, 1048 – −1050(1979).

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.