

AuCN Structure: ABC_hP3_183_a_a_a-001

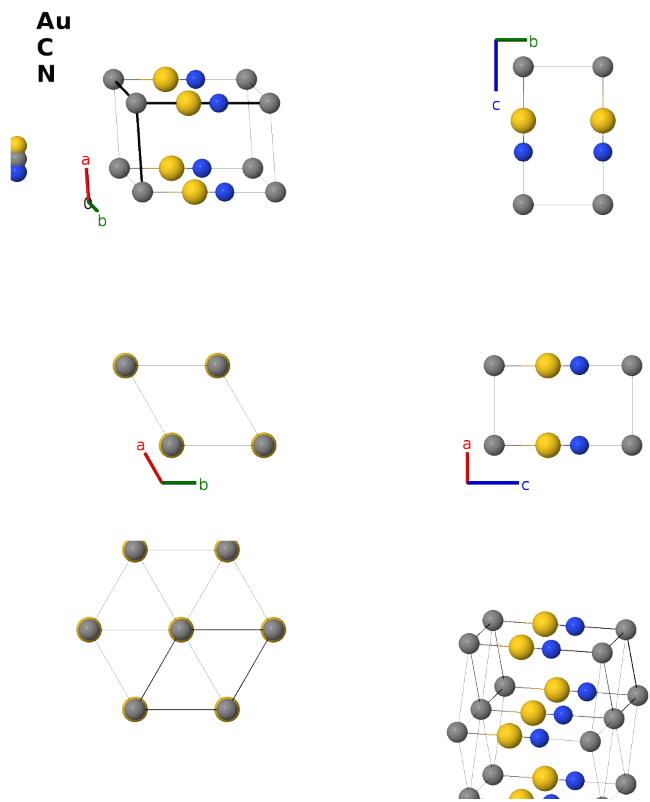
This structure previously used the label(s) **ABC_hP3_183_a_a_a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/Q8EL>

https://aflow.org/prototype-encyclopedia/ABC_hP3_183_a_a_a-001

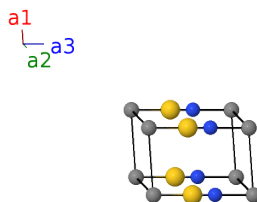


Prototype	AuCN
AFLOW prototype label	ABC_hP3_183_a_a_a-001
ICSD	165175
CCDC	1681240
Pearson symbol	hP3
Space group number	183
Space group symbol	$P6mm$
AFLOW prototype command	<code>aflow --proto=ABC_hP3_183_a_a_a-001 --params=a, c/a, z₁, z₂, z₃</code>

- We use the data taken by (Hibble, 2004) at 300K.
- Space group $P6mm$ #183 allows an arbitrary choice for the origin of the z -axis. Here we set the origin so that $z_2 = 0$ for the carbon (1a) site.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(1a)	Au I
$\mathbf{B}_2$	$= z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(1a)	C I
$\mathbf{B}_3$	$= z_3 \mathbf{a}_3$	$=$	$cz_3 \hat{\mathbf{z}}$	(1a)	N I

References

- [1] S. J. Hibble, A. C. Hannon, and S. M. Cheyne, *Structure of AuCN Determined from Total Neutron Diffraction*, Inorg. Chem. **42**, 4724–4730 (2003), doi:10.1021/ic0342043.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

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