AuCN Structure: ABC_hP3_183_a_a_a-001

This structure originally had the label `ABC_hP3_183_a_a_a`. Calls to that address will be redirected here.

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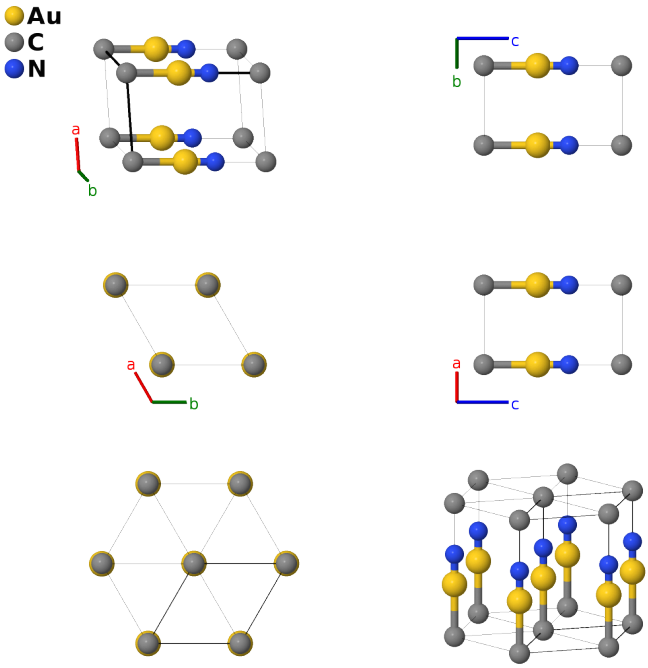
https://aflow.org/p/Q8EL

https://aflow.org/p/ABC_hP3_183_a_a_a-001

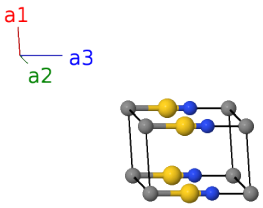


Prototype	AuCN
AFLOW prototype label	ABC_hP3_183_a_a_a-001
ICSD	165175
Pearson symbol	hP3
Space group number	183
Space group symbol	$P6mm$
AFLOW prototype command	`aflow --proto=ABC_hP3_183_a_a_a-001 --params=`$a, c/a, z_1, z_2, z_3$

- 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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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.