

Na₃As (*D*₀₁₈) Structure: AB3_hP8_194_c_bf-001

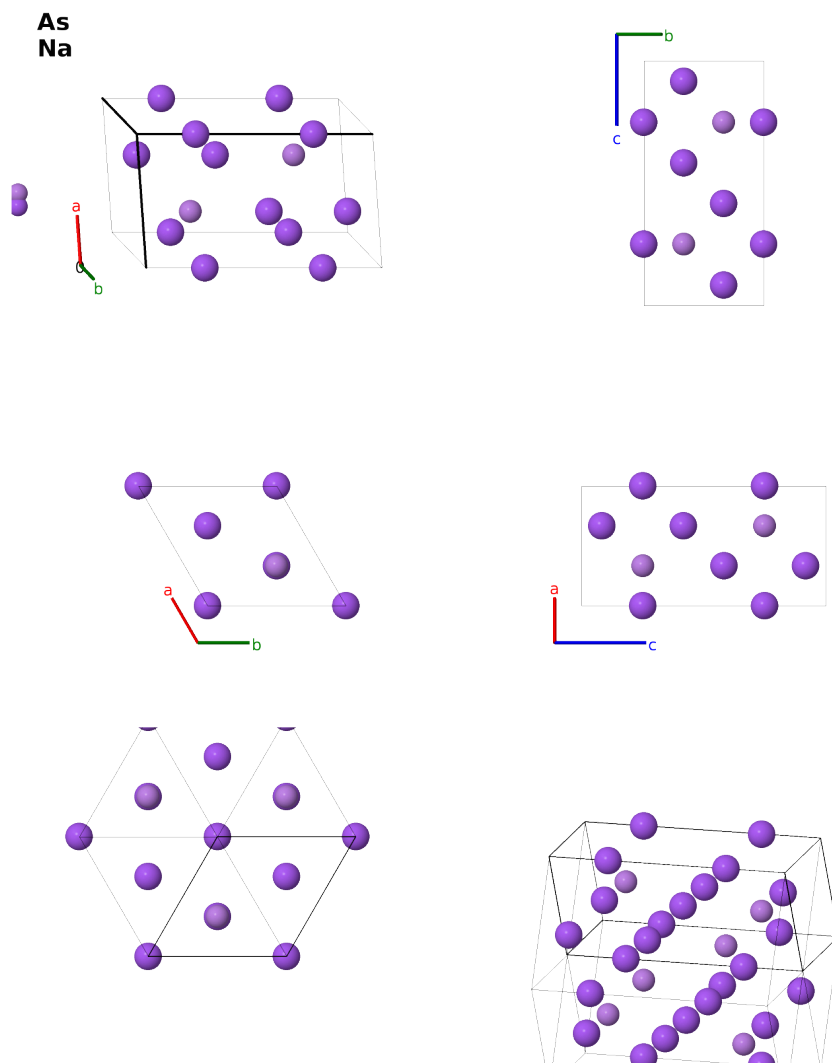
This structure previously used the label(s) **AB3_hP8_194_c_bf**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/5M89>

https://aflow.org/prototype-encyclopedia/AB3_hP8_194_c_bf-001



Prototype	AsNa ₃
AFLOW prototype label	AB3_hP8_194_c_bf-001
Strukturbericht designation	<i>D</i> ₀₁₈
ICSD	26883

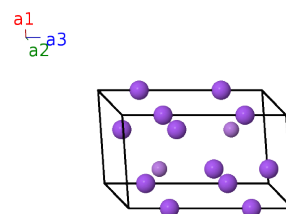
CCDC	1602255
Pearson symbol	hP8
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=AB3_hP8_194_c_bf-001</code> <code>--params=a, c/a, z₃</code>

Other compounds with this structure

K₃As, K₃P, K₃Sb, Li₃As, Mg₃Au, Mg₃Ir, Mg₃Pd, Mg₃Pt, Mg₃Si, Na₃Bi, Na₃P, Na₃Sb, Rb₃As, Rb₃Bi, Rb₃Sb, K₂NaSb

- (Hafner, 1994) argue that the correct structure for Na₃As is not this one, but instead the Cu₃P structure, A3B_hP24_185_ab2c_c, space group $P6_3cm$ #185.

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
$\mathbf{B}_1$	$= \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}c\hat{\mathbf{z}}$	(2b)	Na I
$\mathbf{B}_2$	$= \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}c\hat{\mathbf{z}}$	(2b)	Na I
$\mathbf{B}_3$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(2c)	As I
$\mathbf{B}_4$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(2c)	As I
$\mathbf{B}_5$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + z_3\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$	(4f)	Na II
$\mathbf{B}_6$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + (z_3 + \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + c(z_3 + \frac{1}{2})\hat{\mathbf{z}}$	(4f)	Na II
$\mathbf{B}_7$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 - z_3\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - cz_3\hat{\mathbf{z}}$	(4f)	Na II
$\mathbf{B}_8$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 - (z_3 - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - c(z_3 - \frac{1}{2})\hat{\mathbf{z}}$	(4f)	Na II

References

- [1] P. Hafner and K.-J. Range, *Na₃As revisited: high-pressure synthesis of single crystals and structure refinement*, J. Alloys Compd. **216**, 7–10 (1994), doi:10.1016/0925-8388(94)91033-2.
- [2] G. Brauer and E. Zintl, *Konstitution von Phosphiden, Arseniden, Antimoniden und Wismutiden des Lithiums, Natriums und Kaliums*, Z. Phys. Chem. **37B**, 323–352 (1937).

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.

First cited in

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