

Na₃As Structure:

AB3_hP24_185_c_ab2c-001

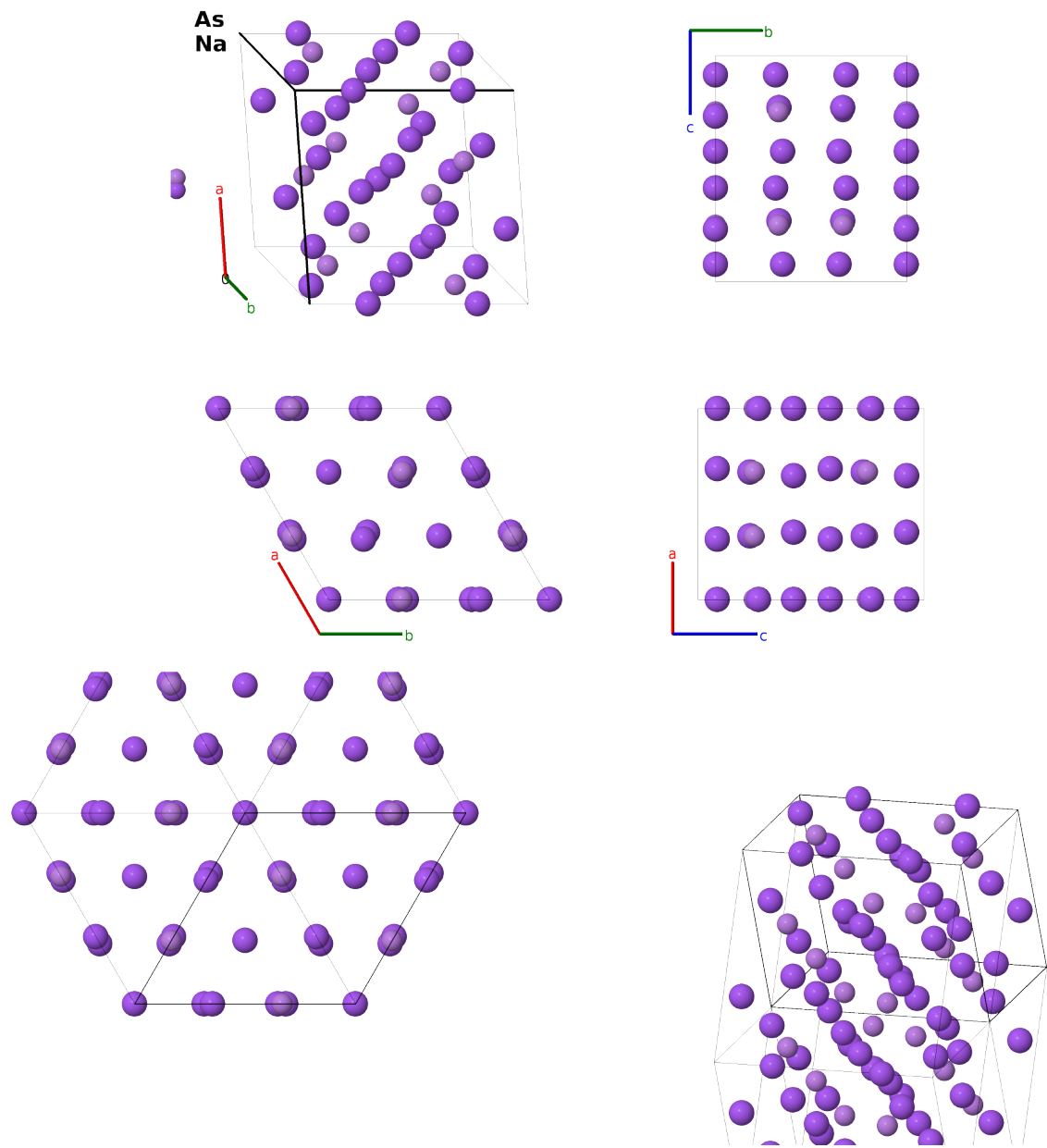
This structure previously used the label(s) **AB3_hP24_185_c_ab2c**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/3ERL>

https://aflow.org/prototype-encyclopedia/AB3_hP24_185_c_ab2c-001



Prototype

AsNa₃

AFLOW prototype label	AB3_hP24_185_c_ab2c-001
ICSD	79586
CCDC	1639832
Pearson symbol	hP24
Space group number	185
Space group symbol	$P6_3cm$
AFLOW prototype command	aflow --proto=AB3_hP24_185_c_ab2c-001 --params= $a, c/a, z_1, z_2, x_3, z_3, x_4, z_4, x_5, z_5$

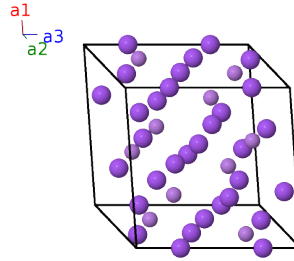
Other compounds with this structure

Cu₃P

- (Hafner, 1994) state that this is a correction of the $D0_{18}$ Na₃As structure, but see the discussion about Cu₃P and other similar compounds.
- Space group $P6_3cm$ #185 allows an arbitrary choice of the origin of the z -axis. Here we set $z_3 = 1/4$ for the arsenic (6c) atoms.

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
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	Na I
$\mathbf{B}_2$	$= \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2a)	Na I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(4b)	Na II
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4b)	Na II
$\mathbf{B}_5$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4b)	Na II
$\mathbf{B}_6$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(4b)	Na II
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a x_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(6c)	As I
$\mathbf{B}_8$	$= x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a x_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(6c)	As I
$\mathbf{B}_9$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + c z_3 \hat{\mathbf{z}}$	(6c)	As I
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a x_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a x_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	As I
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a x_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a x_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	As I
$\mathbf{B}_{12}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	As I

$\mathbf{B}_{13}$	$=$	$x_4 \mathbf{a}_1 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6c)	Na III
$\mathbf{B}_{14}$	$=$	$x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6c)	Na III
$\mathbf{B}_{15}$	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + cz_4 \hat{\mathbf{z}}$	(6c)	Na III
$\mathbf{B}_{16}$	$=$	$-x_4 \mathbf{a}_1 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	Na III
$\mathbf{B}_{17}$	$=$	$-x_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	Na III
$\mathbf{B}_{18}$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	Na III
$\mathbf{B}_{19}$	$=$	$x_5 \mathbf{a}_1 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6c)	Na IV
$\mathbf{B}_{20}$	$=$	$x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6c)	Na IV
$\mathbf{B}_{21}$	$=$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + cz_5 \hat{\mathbf{z}}$	(6c)	Na IV
$\mathbf{B}_{22}$	$=$	$-x_5 \mathbf{a}_1 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_5 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	Na IV
$\mathbf{B}_{23}$	$=$	$-x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_5 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	Na IV
$\mathbf{B}_{24}$	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(6c)	Na IV

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] O. Olofsson, *The Crystal Structure of Cu₃P*, Acta Chem. Scand. **26**, 2777–2787 (1972), doi:10.3891/acta.chem.scand.26-2771.

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