Na_3As Structure: AB3_hP24_185_c_ab2c-001

This structure originally had the label `AB3_hP24_185_c_ab2c`. Calls to that address will be redirected here.

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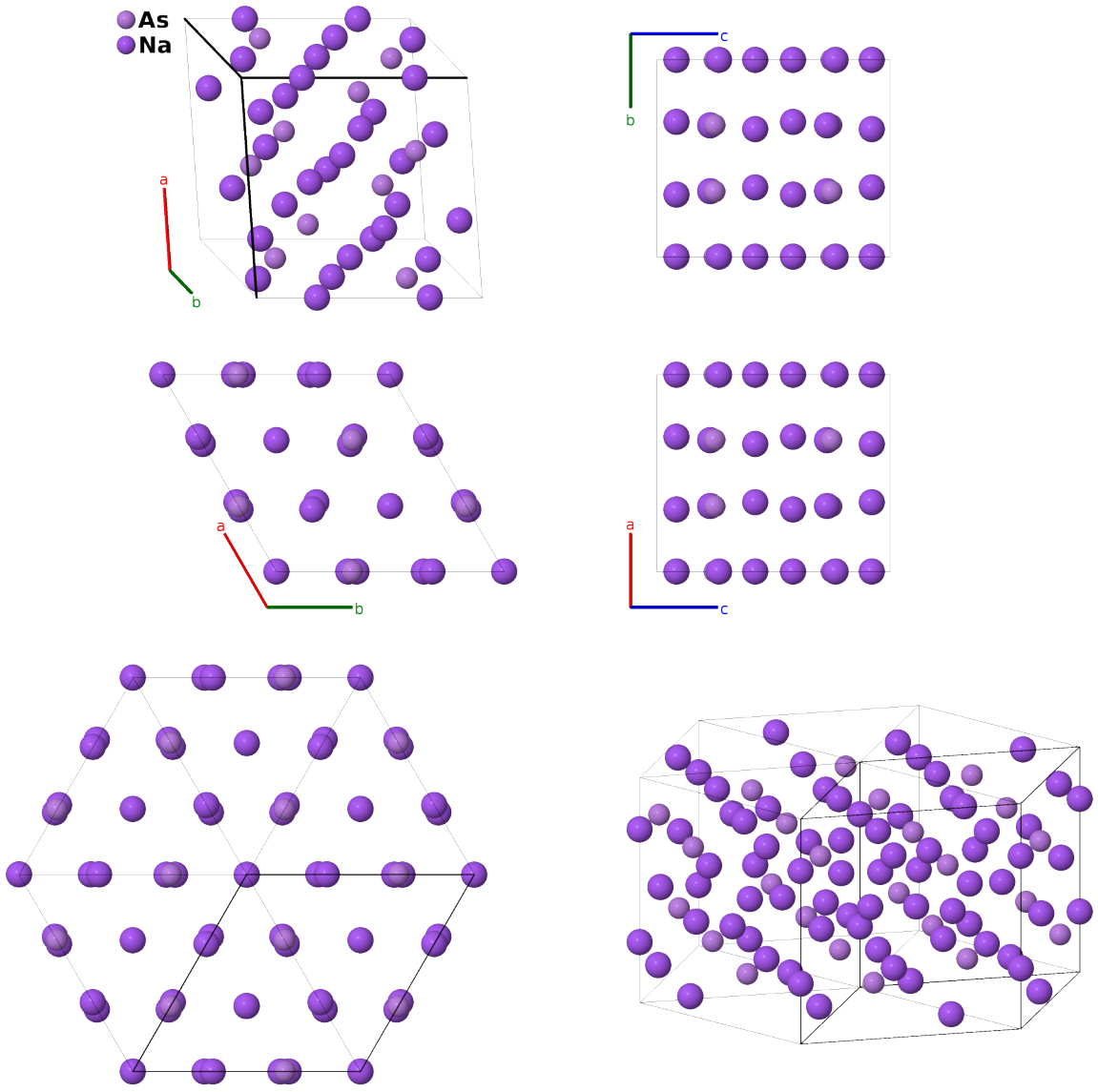
https://aflow.org/p/3ERL

https://aflow.org/p/AB3_hP24_185_c_ab2c-001



Prototype	$AsNa_3$
AFLOW prototype label	AB3_hP24_185_c_ab2c-001
ICSD	79586
Pearson symbol	hP24

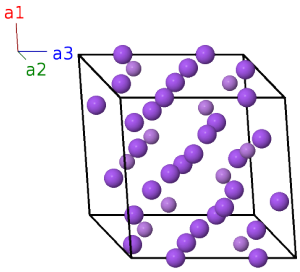
Space group number	185
Space group symbol	$P6_3cm$
AFLOW prototype command	`aflow --proto=AB3_hP24_185_c_ab2c-001 --params=`$a, c/a, z_1, z_2, x_3, z_3, x_4, z_4, x_5, z_5$

Other compounds with this structure
Cu_3P

- (Hafner, 1994) state that this is a correction of the $D0_{18}$ Na_3As structure, but see the discussion about Cu_3P and other similar compounds.
- Space group $P6_3cm$ #185 allows an arbitary choice of the origin of the z-axis. Here we set $z_3 = 1/4$ for the arsenic (6c) atoms.

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
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(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
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(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
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(4b)	Na II
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(6c)	As I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(6c)	As I
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1-x_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}+cz_3\,\hat{\mathbf{z}}$	(6c)	As I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	As I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	As I
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a}_1+x_3\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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

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[2] O. Olofsson, *The Crystal Structure of Cu_3P*, Acta Chem. Scand. **26**, 2777–2787 (1972), doi:10.3891/acta.chem.scand.26-2771.