

AsTi (B_i) Structure: AB_hP8_194_ac_f-004

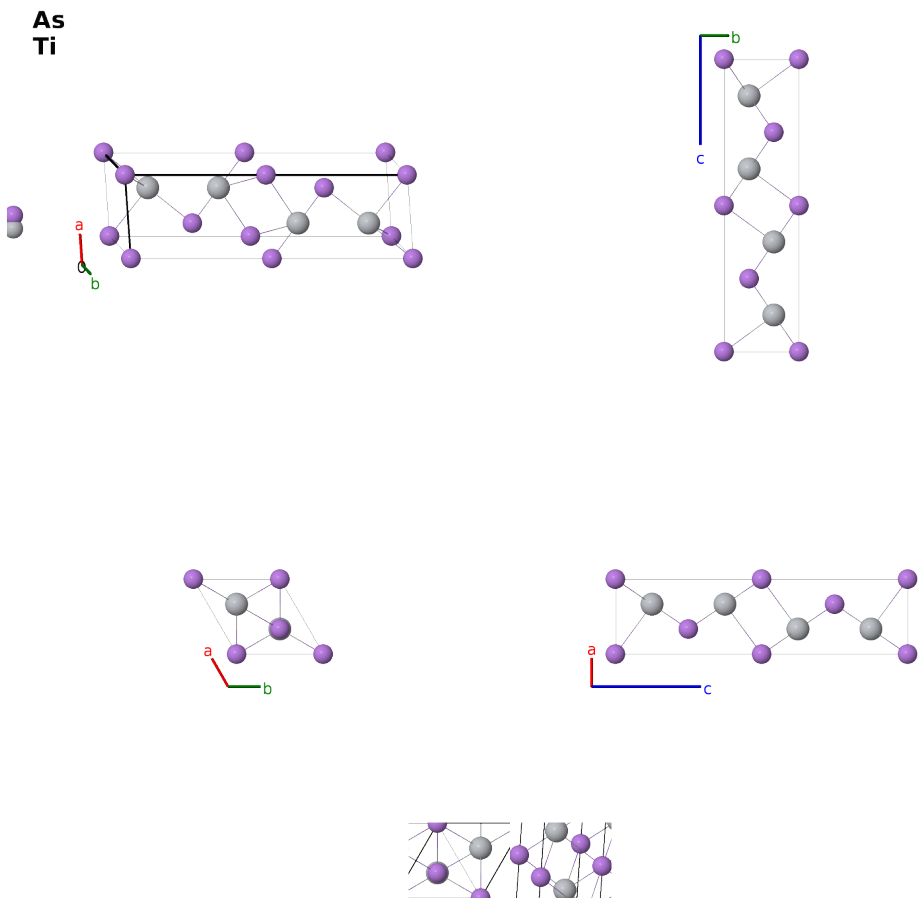
This structure previously used the label(s) **AB_hP8_194_ad_f**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/E9RV>

https://aflow.org/prototype-encyclopedia/AB_hP8_194_ac_f-004



Prototype	AsTi
AFLOW prototype label	AB_hP8_194_ac_f-004
<i>Strukturbericht</i> designation	B_i
ICSD	16773
CCDC	1597322
Pearson symbol	hP8
Space group number	194

Space group symbol $P6_3/mmc$

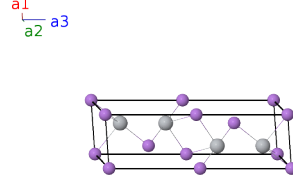
AFLOW prototype command `aflow --proto=AB_hP8_194_ac_f-004`
`--params=a,c/a,z3`

Other compounds with this structure

AsHf, AsZr, CMO, CRe, CSTi₂, CSZr₂, NNb, NW, PTi, PZr, STi, (Ta_{0.75}Mn_{0.25})N

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
$\mathbf{B}_1$	$= 0$	$=$	0	(2a)	As I
$\mathbf{B}_2$	$= \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}c\hat{\mathbf{z}}$	(2a)	As 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 II
$\mathbf{B}_4$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(2c)	As II
$\mathbf{B}_5$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + z_3\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$	(4f)	Ti I
$\mathbf{B}_6$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + (z_3 + \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + c(z_3 + \frac{1}{2})\hat{\mathbf{z}}$	(4f)	Ti I
$\mathbf{B}_7$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 - z_3\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - cz_3\hat{\mathbf{z}}$	(4f)	Ti I
$\mathbf{B}_8$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 - (z_3 - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - c(z_3 - \frac{1}{2})\hat{\mathbf{z}}$	(4f)	Ti I

References

- [1] K. Bachmayer, H. Nowotny, and A. Kohl, *Die Struktur von TiAs*, Monatsh. Chem. Verw. Tl. **86**, 39–43 (1955), doi:10.1007/BF00899271.

Found in

- [1] R. G. W. Wyckoff, *Crystal Structure*, vol. 1 (Interscience, New York, London, Sydney, 1963).

First cited in

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