

α -As (A7) Structure: A_hR2_166_c-001

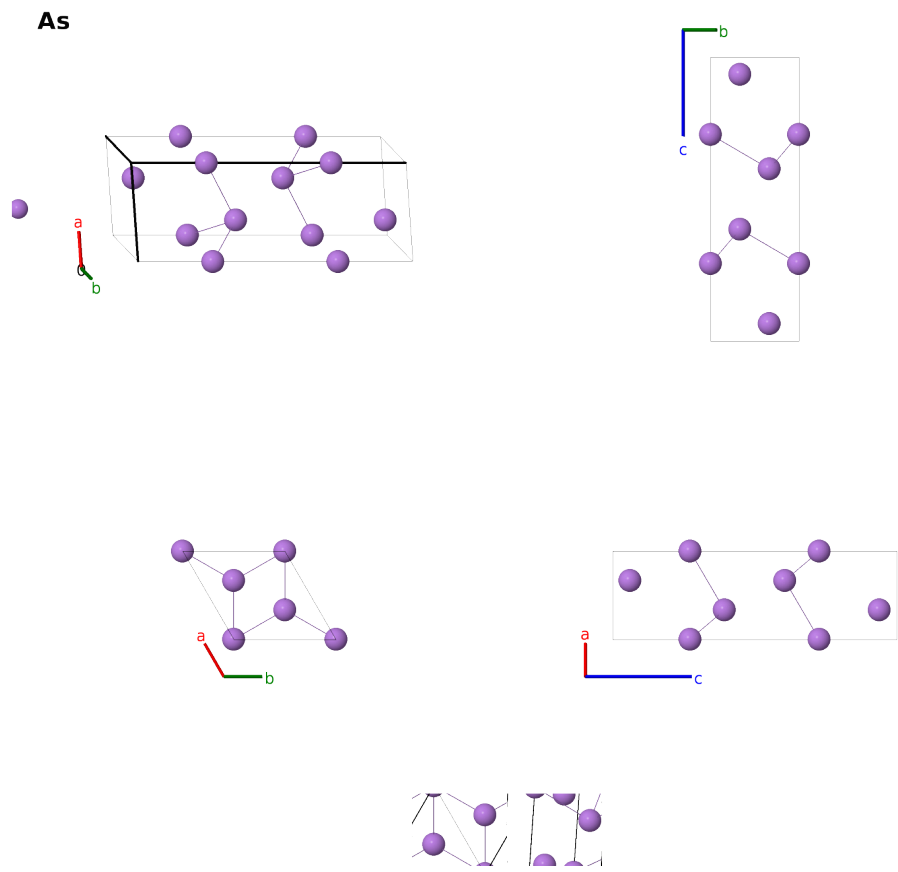
This structure previously used the label(s) **A_hR2_166_c.alpha-As**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/F2V5>

https://aflow.org/prototype-encyclopedia/A_hR2_166_c-001



Prototype	As
AFLOW prototype label	A_hR2_166_c-001
<i>Strukturbericht</i> designation	A7
ICSD	16517
CCDC	1597091
Pearson symbol	hR2
Space group number	166
Space group symbol	$R\bar{3}m$

AFLOW prototype command `aflow --proto=A_hR2_166_c-001`
 `--params=a, c/a, x1`

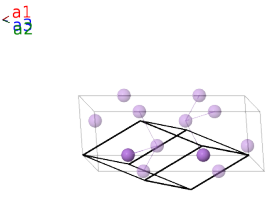
Other compounds with this structure

Bi, Sb

- We use the data from (Schiferl, 1969) taken at 78K.
- When $c/a = \sqrt{6}$ and $z_1 = 1/8$ this becomes the diamond (A4) structure.
- Note that α -As (A7), rhombohedral graphite (A_hR2_166_c), and β -O have the same AFLOW prototype label, A_hR2_166_c. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files. Hexagonal settings of rhombohedral structures can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$cx_1 \hat{\mathbf{z}}$	(2c) As I
$\mathbf{B}_2$	$=$	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-cx_1 \hat{\mathbf{z}}$	(2c) As I

References

- [1] D. Schiferl and C. S. Barrett, *The crystal structure of arsenic at 4.2, 78 and 299 K*, J. Appl. Crystallogr. **2**, 30–36 (1969), doi:10.1107/S0021889869006443.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017