α-As ($A7$) Structure: A_hR2_166_c-001

This structure originally had the label `A_hR2_166_c.alpha-As`. Calls to that address will be redirected here.

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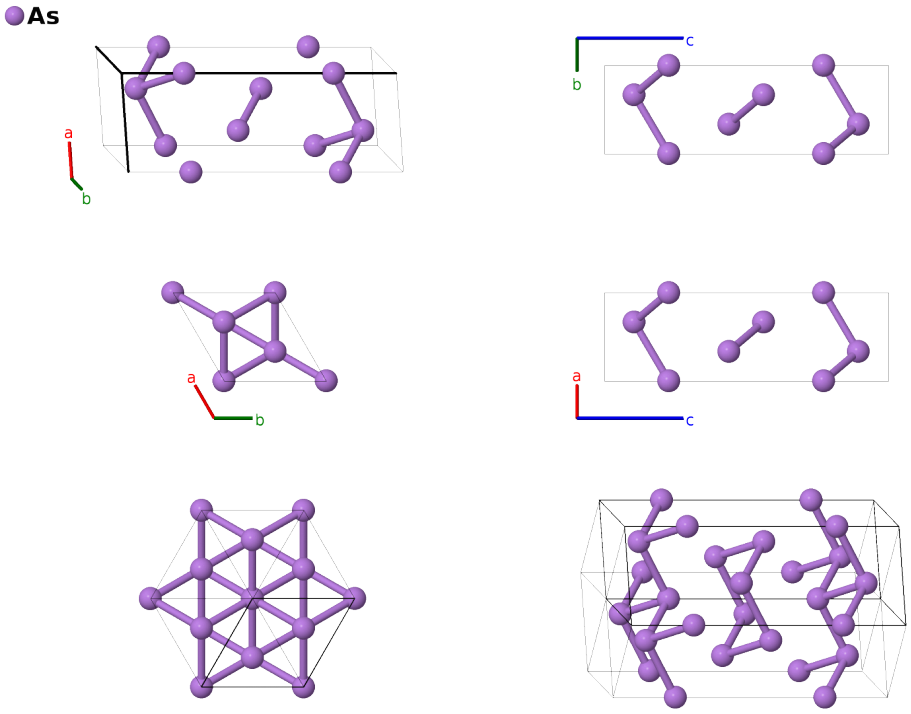
https://aflow.org/p/F2V5

https://aflow.org/p/A_hR2_166_c-001



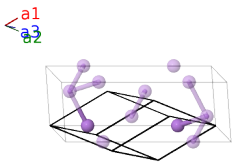
Prototype	As
AFLOW prototype label	A_hR2_166_c-001
***Strukturbericht* designation**	$A7$
ICSD	16517
Pearson symbol	hR2
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A_hR2_166_c-001 --params=`$a, c/a, x_1$

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

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$



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).