

V₃AsC Structure: ABC3_oC20_63_c_a_cf-003

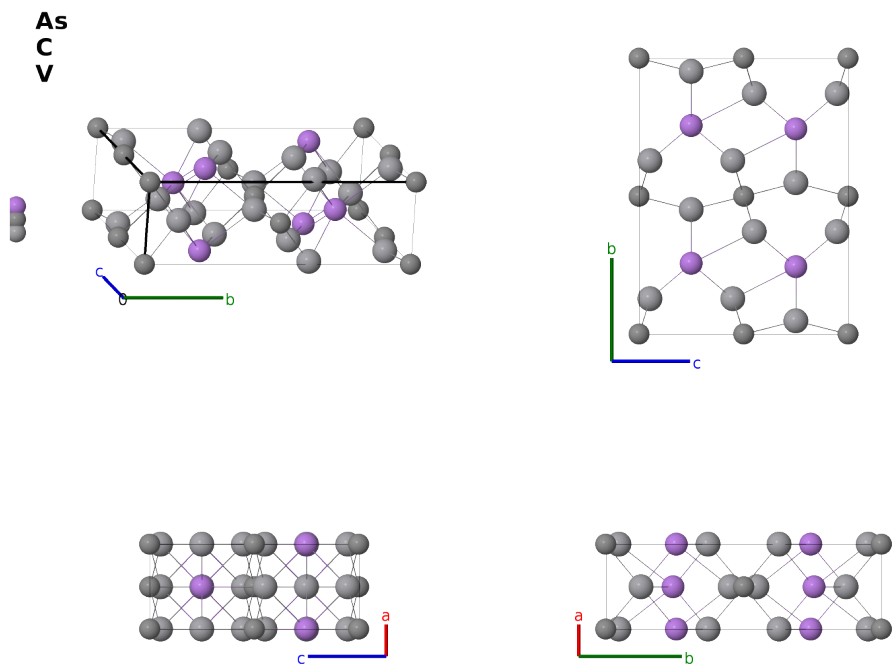
This structure previously used the label(s) **ABC3_oC20_63_c_b_cf**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/2T8B>

https://aflow.org/prototype-encyclopedia/ABC3_oC20_63_c_a_cf-003



Prototype	AsCV ₃
AFLOW prototype label	ABC3_oC20_63_c_a_cf-003
ICSD	25761
CCDC	1601404
Pearson symbol	oC20
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=ABC3_oC20_63_c_a_cf-003</code> <code>--params=a, b/a, c/a, y₂, y₃, y₄, z₄</code>

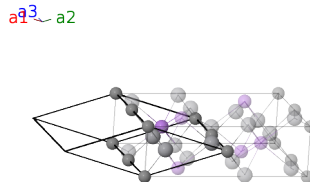
Other compounds with this structure

V₃PC, V₃PN, V₃AsN, Cr₃PC, Cr₃AsC, Zr₃AlN, UScS₃

- This structure is a “filled” version of the Re₃B structure, with carbon atoms sitting in the (4b) Wyckoff positions. This is the ternary version of the structure. The quaternary version, where all Wyckoff positions contain different species of atoms, is listed as the ThFe₂SiC structure.
- We have shifted the origin to move the first of the C I atoms to the origin.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(4a) C I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}c \hat{\mathbf{z}}$	(4a) C I
$\mathbf{B}_3$	=	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c) As I
$\mathbf{B}_4$	=	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$-by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c) As I
$\mathbf{B}_5$	=	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$by_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c) V I
$\mathbf{B}_6$	=	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	=	$-by_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c) V I
$\mathbf{B}_7$	=	$-y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8f) V II
$\mathbf{B}_8$	=	$y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$-by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f) V II
$\mathbf{B}_9$	=	$-y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	=	$by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f) V II
$\mathbf{B}_{10}$	=	$y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8f) V II

References

- [1] H. Boller and H. Nowotny, *Zum Dreistoff: Vanadin-Arsen-Kohlenstoff*, Monatsh. Chem. **98**, 2127–2132 (1967), doi:10.1007/BF01167176.

Found in

- [1] A. M. Witte and W. Jeitschko, *Carbides with Filled Re₃B-Type Structure*, J. Solid State Chem. **112**, 232–236 (1994), doi:10.1006/jssc.1994.1297.

First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.