V_3AsC Structure: ABC3_oC20_63_c_a_cf-003

This structure originally had the label `ABC3_oC20_63_c_b_cf`. Calls to that address will be redirected here.

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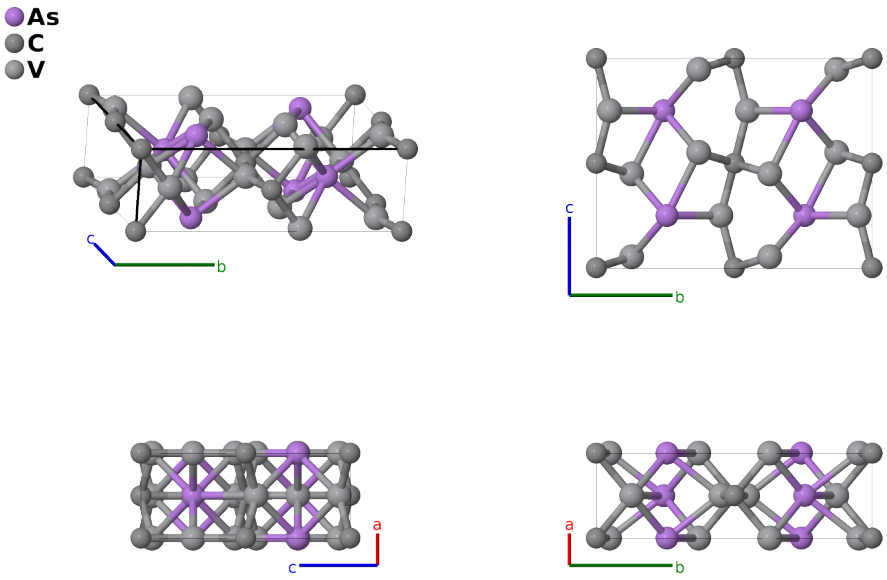
https://aflow.org/p/2T8B

https://aflow.org/p/ABC3_oC20_63_c_a_cf-003



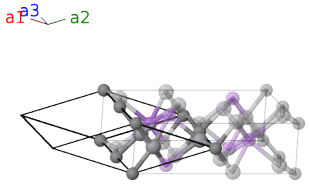
Prototype	$AsCV_3$
AFLOW prototype label	ABC3_oC20_63_c_a_cf-003
ICSD	25761
Pearson symbol	oC20
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=ABC3_oC20_63_c_a_cf-003 --params=`$a, b/a, c/a, y_2, y_3, y_4, z_4$

Other compounds with this structure
V_3PC, V_3PN, V_3AsN, Cr_3PC, Cr_3AsC, Zr_3AlN, $UScS_3$

- This structure is a "filled" version of the Re_3B 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 $ThFe_2SiC$ structure.
- We have shifted the origin to move the first of the C I atoms to the origin.

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_8}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	V II
$\mathbf{B_9}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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 Re_3B-Type Structure*, J. Solid State Chem. **112**, 232–236 (1994), doi:10.1006/jssc.1994.1297.