Ta_2VC_2 Structure: A3B2C_hR6_166_ac_c_b-001

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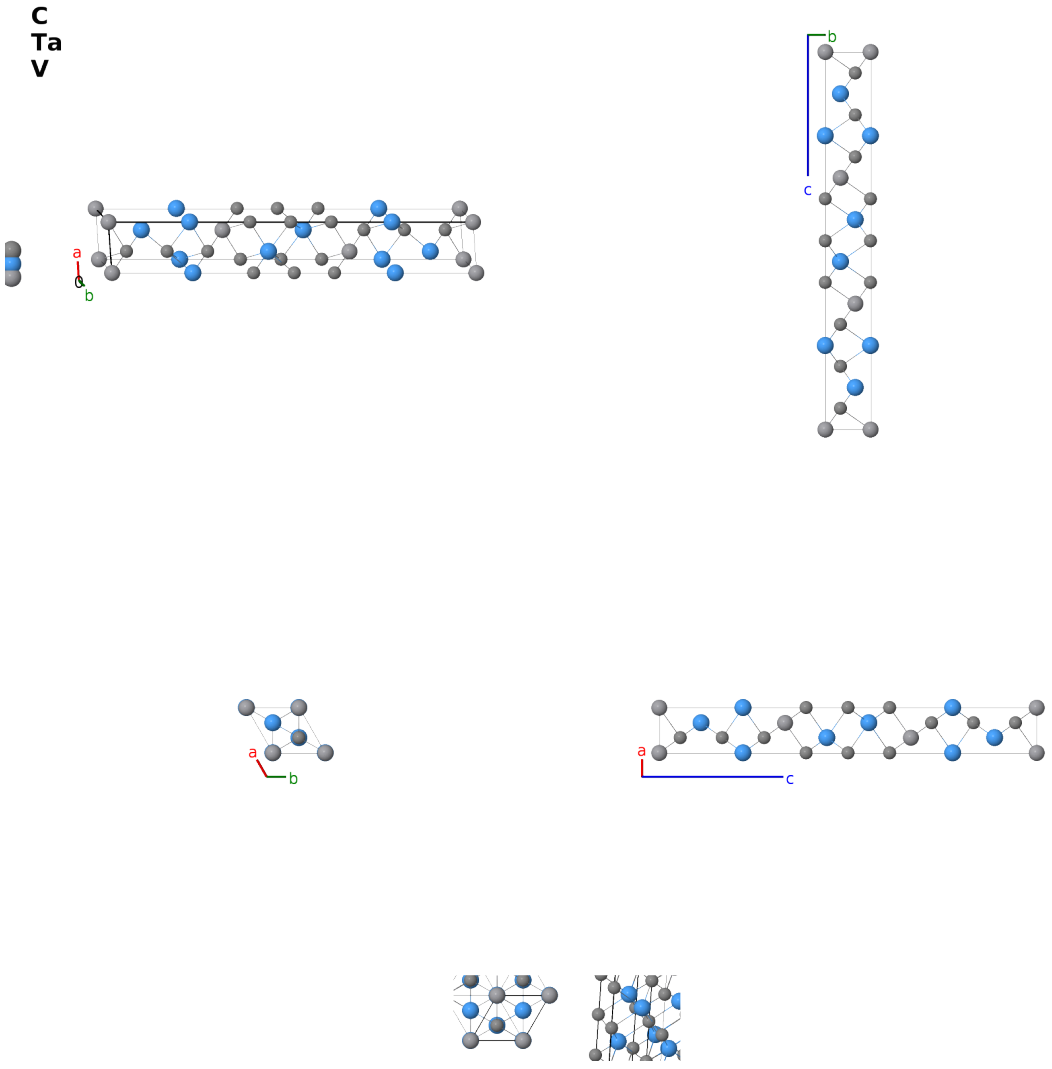
https://aflow.org/prototype-encyclopedia/FC27

https://aflow.org/prototype-encyclopedia/A3B2C_hR6_166_ac_c_b-001



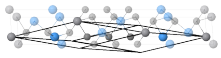
Prototype	C_2TaV
AFLOW prototype label	A3B2C_hR6_166_ac_c_b-001
ICSD	23570
CCDC	1599676
Pearson symbol	hR6

Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A3B2C_hR6_166_ac_c_b-001 --params=`$a, c/a, x_3, x_4$

- All of the sites here are in some way disordered:
- The (1a) site is 2/3 tantalum and 1/3 vanadium. We have arbitrarily labeled this as vanadium.
- The C I (1b) and C II (2c) sites are occupied 2/3 of the time.
- The second (2c) site is also 2/3 tantalum and 1/3 vanadium, and we have arbitrarily labeled it as tantalum.
- ϵ-Hf_3N_2 is the binary form of this structure.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	C I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	V I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	C II
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	C II
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(2c)	Ta I
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-cx_4\,\hat{\mathbf{z}}$	(2c)	Ta I

References

[1] E. Rudy, *The crystal structure of Ta_2VC_2* **49**, 49–55 (1970), doi:10.1016/0022-5088(70)90035-4.

Found in

[1] E. Rudy, *The Crystal Structures of Hf_3N_2 and Hf_4N_3*, Metall. Trans. **1**, 1249–1252 (1970), doi:10.1007/BF02900238.

First cited in

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