KV_3Sb_5 Structure: AB5C3_hP9_191_b_ah_f-001

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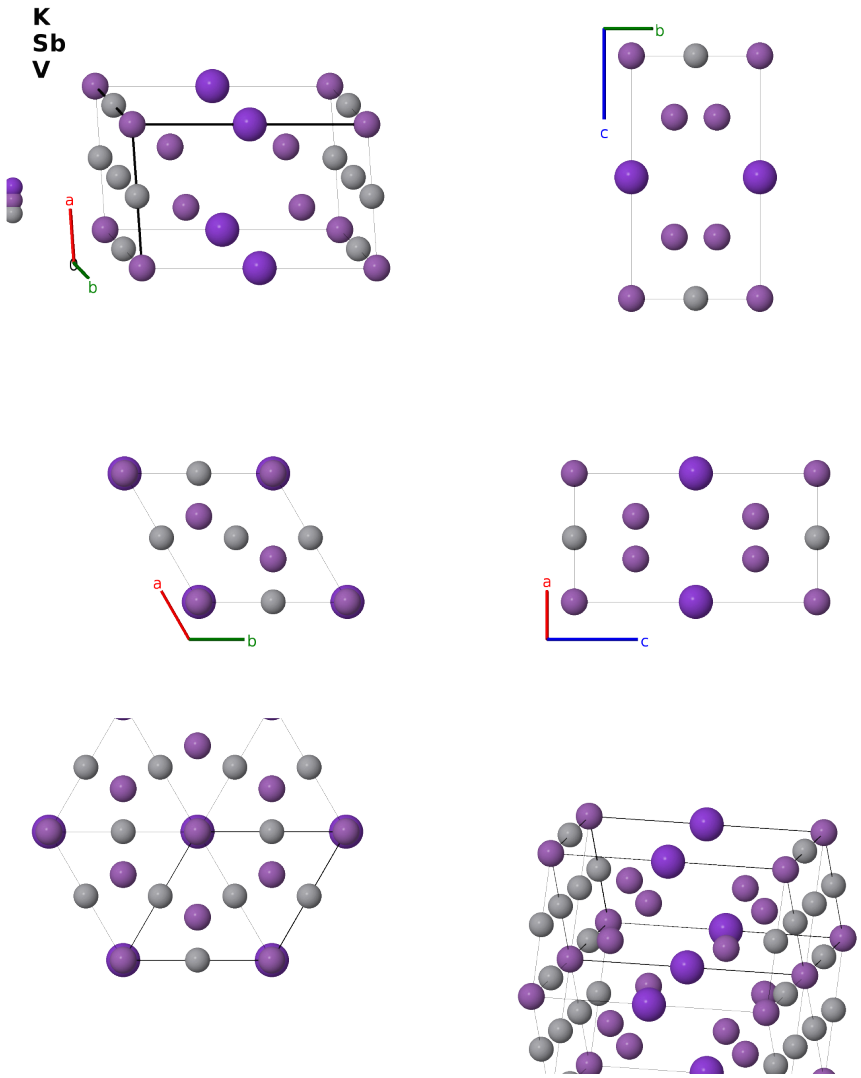
https://aflow.org/prototype-encyclopedia/F3TR

https://aflow.org/prototype-encyclopedia/AB5C3_hP9_191_b_ah_f-001



Prototype	KSb_5V_3
AFLOW prototype label	AB5C3_hP9_191_b_ah_f-001
ICSD	31838
CCDC	2077548
Pearson symbol	hP9

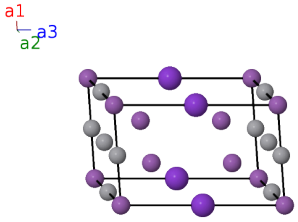
Space group number	191
Space group symbol	$P6/mmm$
AFLOW prototype command	`aflow --proto=AB5C3_hP9_191_b_ah_f-001 --params=`$a, c/a, z_4$

Other compounds with this structure
$CsTi_3Bi_5$, CsV_3Sb_5, RbV_3Sb_5

- (Ortiz, 2019) found that their KV_3Sb_5 samples were potassium deficient, with 8-15% vacancies on the (1a) potassium site. Both CsV_3Sb_5 and RbV_3Sb_5 were stoichiometric.
- This is a kagome structure.

Hexagonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Sb I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	K I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(3f)	V I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(3f)	V I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(3f)	V I
$\mathbf{B_6}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4h)	Sb II
$\mathbf{B_7}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4h)	Sb II
$\mathbf{B_8}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4h)	Sb II
$\mathbf{B_9}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4h)	Sb II

References

[1] B. R. Ortiz, L. C. Gomes, J. R. Morey, M. Winiarski, M. Bordelon, J. S. Mangum, I. W. H. Oswald, J. A. Rodriguez-Rivera, J. R. Neilson, S. D. Wilson, E. Ertekin, T. M. McQueen, and E. S. Toberer, *New kagome prototype materials: discovery of KV_3Sb_5,RbV_3Sb_5, and CsV_3Sb_5*, Phys. Rev. Materials **3**, 094407 (2019), doi:10.1103/PhysRevMaterials.3.094407.

Found in

[1] B. R. Ortiz, S. M. L. Teicher, Y. Hu, J. L. Zuo, P. M. Sarte, E. C. Schueller, A. M. M. Abeykoon, M. J. Krogstad, S. Rosenkranz, R. Osborn, R. Seshadri, L. Balents, J. He, and S. D. Wilson, *CsV_3Sb_5: a Z_2 topological kagome metal with a superconducting ground state*, Phys. Rev. Lett. **125**, 247002 (2020), doi:10.1103/PhysRevLett.125.247002.

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