

CsV₆Sb₆ Structure:

AB6C6_hR13_166_a_3c_h-001

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<https://aflow.org/prototype-encyclopedia/KPVW>

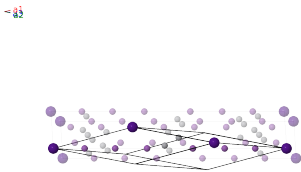
https://aflow.org/prototype-encyclopedia/AB6C6_hR13_166_a_3c_h-001

Prototype	CsSb ₆ V ₆
AFLOW prototype label	AB6C6_hR13_166_a_3c_h-001
Pearson symbol	hR13
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=AB6C6_hR13_166_a_3c_h-001</code> <code>--params=a,c/a,x₂,x₃,x₄,x₅,z₅</code>

- This is a kagome structure.

Rhombohedral primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	Cs I
$\mathbf{B}_2$	$=$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(2c) Sb I
$\mathbf{B}_3$	$=$	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-cx_2 \hat{\mathbf{z}}$	(2c) Sb I
$\mathbf{B}_4$	$=$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$cx_3 \hat{\mathbf{z}}$	(2c) Sb II
$\mathbf{B}_5$	$=$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-cx_3 \hat{\mathbf{z}}$	(2c) Sb II
$\mathbf{B}_6$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$cx_4 \hat{\mathbf{z}}$	(2c) Sb III

$$\begin{aligned}
\mathbf{B}_7 &= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3 &= -cx_4 \hat{\mathbf{z}} & (2c) & \text{Sb III} \\
\mathbf{B}_8 &= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}} & (6h) & \text{V I} \\
\mathbf{B}_9 &= z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3 &= -\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}} & (6h) & \text{V I} \\
\mathbf{B}_{10} &= x_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3 &= -\frac{1}{\sqrt{3}}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}} & (6h) & \text{V I} \\
\mathbf{B}_{11} &= -z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3 &= \frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}} & (6h) & \text{V I} \\
\mathbf{B}_{12} &= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}} & (6h) & \text{V I} \\
\mathbf{B}_{13} &= -x_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3 &= \frac{1}{\sqrt{3}}a(x_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}} & (6h) & \text{V I}
\end{aligned}$$

References

- [1] Q. Yin, Z. Tu, C. Gong, S. Tian, and H. Lei, *Structures and Physical Properties of V-Based Kagome Metals CsV_6Sb_6 and $\text{CsV}_8\text{Sb}_{12}$* , Chinese Phys. Lett. **38**, 127401 (2021), doi:10.1088/0256-307X/38/12/127401.

Found in

- [1] X. Liu, X. Zhang, J. Jiao, R. Zhang, K. Chen, Y. Wang, Y. Ye, Z. Yu, C. Jiang, X. Wang, L. Shu, B. Lv, G. Li, and Y. Guo, *Emergent dynamical Kondo coherence and competing magnetic order in a correlated kagome flat-band metal CsCr_6Sb_6* (2025), doi:10.48550/arXiv.2508.08580. ArXiv:2508.08580 [cond-mat.str-el].

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Cs
Sb
V

