

Cr-233 Quasi-One-Dimensional Superconductor ($\text{K}_2\text{Cr}_3\text{As}_3$) Structure:

A3B3C2_hP16_187_jk_jk_ak-001

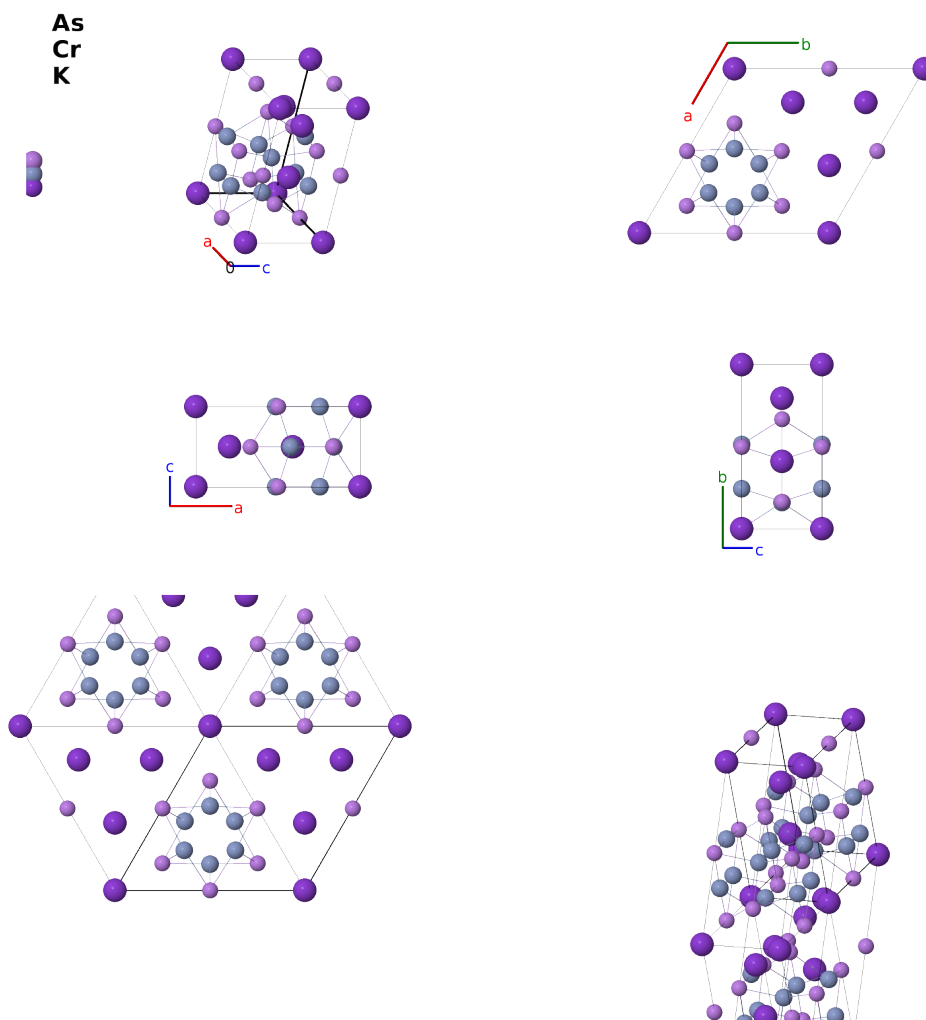
This structure previously used the label(s) **A3B3C2_hP16_187_jk_jk_ck**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/XP6Z>

https://aflow.org/prototype-encyclopedia/A3B3C2_hP16_187_jk_jk_ak-001



Prototype

$\text{As}_3\text{Cr}_3\text{K}_2$

AFLOW prototype label

A3B3C2_hP16_187_jk_jk_ak-001

ICSD

35909

CCDC	2197457
Pearson symbol	hP16
Space group number	187
Space group symbol	$P\bar{6}m2$
AFLOW prototype command	aflow --proto=A3B3C2_hP16_187_jk_jk_ak-001 --params= $a, c/a, x_2, x_3, x_4, x_5, x_6$

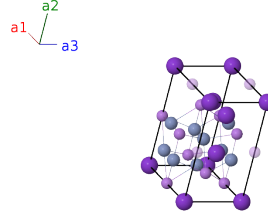
Other compounds with this structure

$\text{Cs}_2\text{Cr}_3\text{As}_3$, $\text{K}_2\text{Mo}_3\text{As}_3$, $\text{Rb}_2\text{Cr}_3\text{As}_3$, $\text{Rb}_2\text{Mo}_3\text{As}_3$

- Cr-233 designates a class of structures of the form $\text{A}_2\text{B}_2\text{As}_3$, where the “A” atoms form one-dimensional chains. Several of these compounds have been found to superconduct at temperatures on the order of 5-10K.
- The ICSD entry is for $\text{Rb}_2\text{Mo}_3\text{As}_3$ from (Zhao, 2020). The ICSD entry lists that as the prototype, but (Bao, 2015) obviously found $\text{K}_2\text{Cr}_3\text{As}_3$ earlier, so we continue using it as our prototype.

Hexagonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(1a)	K I
$\mathbf{B}_2$	$= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-\sqrt{3}ax_2\hat{\mathbf{y}}$	(3j)	As I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2$	$=$	$\frac{3}{2}ax_2\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\hat{\mathbf{y}}$	(3j)	As I
$\mathbf{B}_4$	$= -2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$-\frac{3}{2}ax_2\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\hat{\mathbf{y}}$	(3j)	As I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-\sqrt{3}ax_3\hat{\mathbf{y}}$	(3j)	Cr I
$\mathbf{B}_6$	$= x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2$	$=$	$\frac{3}{2}ax_3\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}}$	(3j)	Cr I
$\mathbf{B}_7$	$= -2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-\frac{3}{2}ax_3\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\hat{\mathbf{y}}$	(3j)	Cr I
$\mathbf{B}_8$	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$-\sqrt{3}ax_4\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(3k)	As II
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{3}{2}ax_4\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(3k)	As II
$\mathbf{B}_{10}$	$= -2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_4\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(3k)	As II
$\mathbf{B}_{11}$	$= x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$-\sqrt{3}ax_5\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(3k)	Cr II
$\mathbf{B}_{12}$	$= x_5 \mathbf{a}_1 + 2x_5 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{3}{2}ax_5\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(3k)	Cr II
$\mathbf{B}_{13}$	$= -2x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_5\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(3k)	Cr II
$\mathbf{B}_{14}$	$= x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$-\sqrt{3}ax_6\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(3k)	K II
$\mathbf{B}_{15}$	$= x_6 \mathbf{a}_1 + 2x_6 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{3}{2}ax_6\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(3k)	K II
$\mathbf{B}_{16}$	$= -2x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$-\frac{3}{2}ax_6\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$	(3k)	K II

References

- [1] J.-K. Bao, J.-Y. Liu, C.-W. Ma, Z.-H. Meng, Z.-T. Tang, Y.-L. Sun, H.-F. Zhai, H. Jiang, H. Bai, C.-M. Feng, Z.-A. Xu, and G.-H. Cao, *Superconductivity in Quasi-One-Dimensional $K_2Cr_3As_3$ with Significant Electron Correlations*, Phys. Rev. X **5**, 011013 (2015), doi:10.1103/PhysRevX.5.011013.
- [2] K. Zhao, Q.-G. Mu, B.-B. Ruan, M.-H. Zhou, Q.-S. Yang, T. Liu, B.-J. Pan, S. Zhang, G.-F. Chen, and Z.-A. Ren, *A New Quasi-One-Dimensional Ternary Molybdenum Pnictide $Rb_2Mo_3As_3$ with Superconducting Transition at 10.5K*, Chin. Phys. Lett. **37**, 097401 (2020), doi:10.1088/0256-307X/37/9/097401.

Found in

- [1] Q.-G. Mu, B.-B. Ruan, K. Zhao, B.-J. Pan, T. Liu, L. Shan, G.-F. Chen, and Z.-A. Ren, *Superconductivity at 10.4 K in a novel quasi-one-dimensional ternary molybdenum pnictide $K_2Mo_3As_3$* , Science Bulletin **63**, 952–956 (2008), doi:10.1016/j.scib.2018.06.011.

First cited in

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