# Cr-233 Quasi-One-Dimensional Superconductor ($K_2Cr_3As_3$) Structure: A3B3C2_hP16_187_jk_jk_ak-001

This structure originally had the label `A3B3C2_hP16_187_jk_jk_ck`. Calls to that address will be redirected here.

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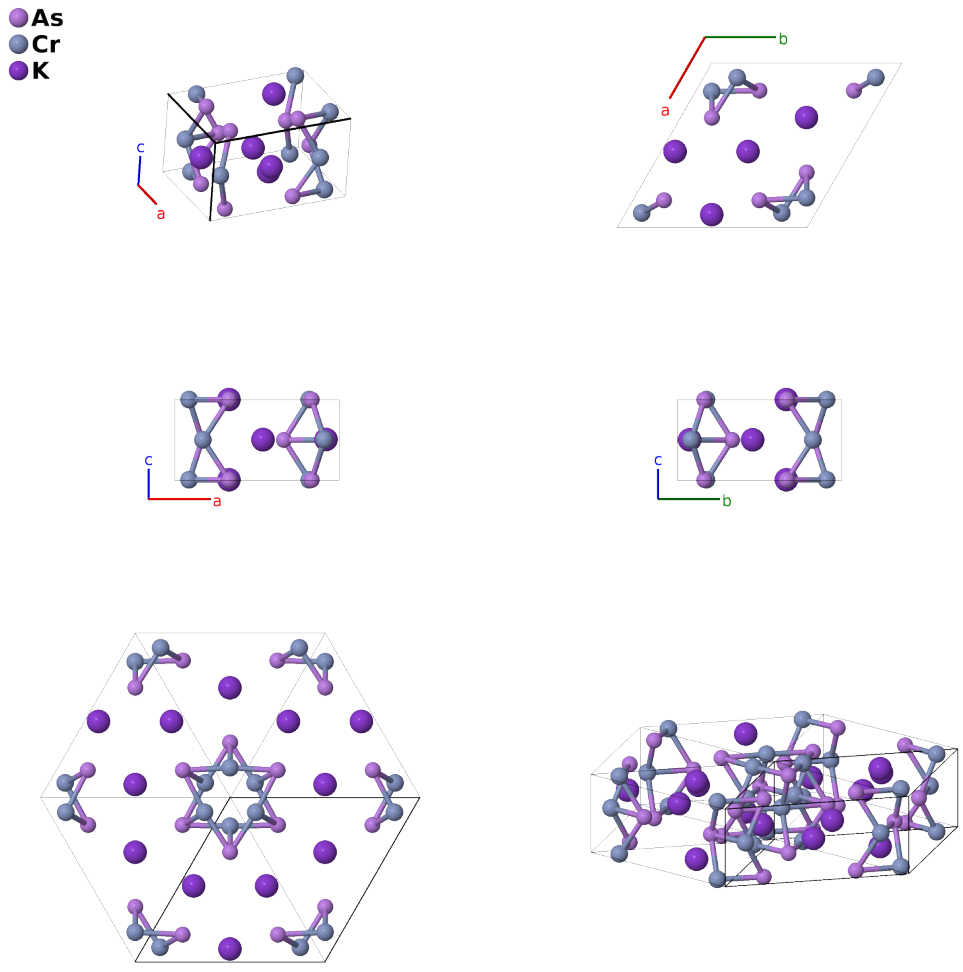
https://aflow.org/p/XP6Z

https://aflow.org/p/A3B3C2_hP16_187_jk_jk_ak-001




| | |
|---|---|
| **Prototype** | $As_3Cr_3K_2$ |
| **AFLOW prototype label** | A3B3C2_hP16_187_jk_jk_ak-001 |
| **ICSD** | 35909 |
| **Pearson symbol** | hP16 |
| **Space group number** | 187 |
| **Space group symbol** | $P\bar{6}m2$ |

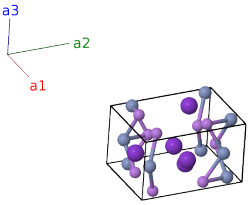
**AFLOW prototype command** `aflow --proto=A3B3C2_hP16_187_jk_jk_ak-001 --params=`$a, c/a, x_2, x_3, x_4, x_5, x_6$

**Other compounds with this structure**
$Cs_2Cr_3As_3$, $K_2Mo_3As_3$, $Rb_2Cr_3As_3$, $Rb_2Mo_3As_3$

- Cr-233 designates a class of structures of the form $A_2B_2As_3$, 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 $Rb_2Mo_3As_3$ from (Zhao, 2020). The ICSD entry lists that as the prototype, but (Bao, 2015) obviously found $K_2Cr_3As_3$ earlier, so we continue using it as our prototype.

**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) | 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.