

CoU (B_a) Structure: AB_cI16_199_a_a-001

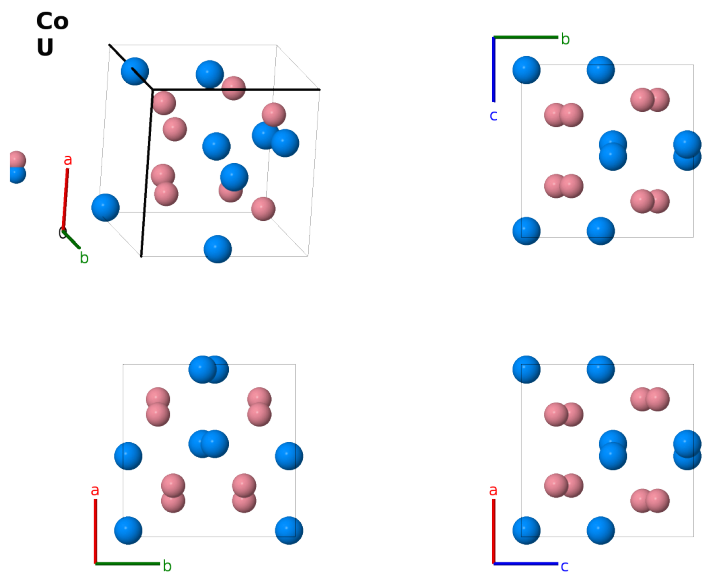
This structure previously used the label(s) **AB_cI16_199_a_a**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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

https://aflow.org/prototype-encyclopedia/AB_cI16_199_a_a-001



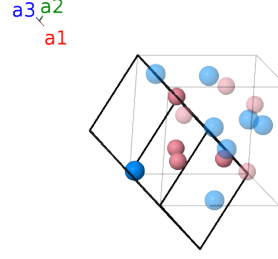
Prototype	CoU
AFLOW prototype label	AB_cI16_199_a_a-001
<i>Strukturbericht</i> designation	B_a
ICSD	102712
CCDC	1660682
Pearson symbol	cI16
Space group number	199
Space group symbol	$I2_13$
AFLOW prototype command	<code>aflow --proto=AB_cI16_199_a_a-001</code> <code>--params=a, x_1, x_2</code>

Other compounds with this structure
 Ga_2Pu_3

- When $x_1 = 1/4$ and $x_2 = 0$, or visa versa, this structure reduces to CsCl (B2) with $a_{B2} = a/2$.

Body-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 2x_1 \mathbf{a}_1 + 2x_1 \mathbf{a}_2 + 2x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(8a)	Co I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 - (2x_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(8a)	Co I
$\mathbf{B}_3$	$= -(2x_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(8a)	Co I
$\mathbf{B}_4$	$= -(2x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(8a)	Co I
$\mathbf{B}_5$	$= 2x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + 2x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8a)	U I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 - (2x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8a)	U I
$\mathbf{B}_7$	$= -(2x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8a)	U I
$\mathbf{B}_8$	$= -(2x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8a)	U I

References

- [1] N. C. Baenziger, R. E. Rundle, A. I. Snow, and A. S. Wilson, *Compounds of uranium with the transition metals of the first long period*, Acta Cryst. **3**, 34–40 (1950), doi:10.1107/S0365110X50000082.

Found in

- [1] F. A. Rough and A. A. Bauer, *Constitution of Uranium and Thorium Alloys* (1958). Report No. BMI-1300, UC-25 Metallurgy and Ceramics, TID-4500, 13th Ed., Rev.

First cited in

- M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017