

CeCu₂ Structure:

AB2_oI12_74_e_h-001

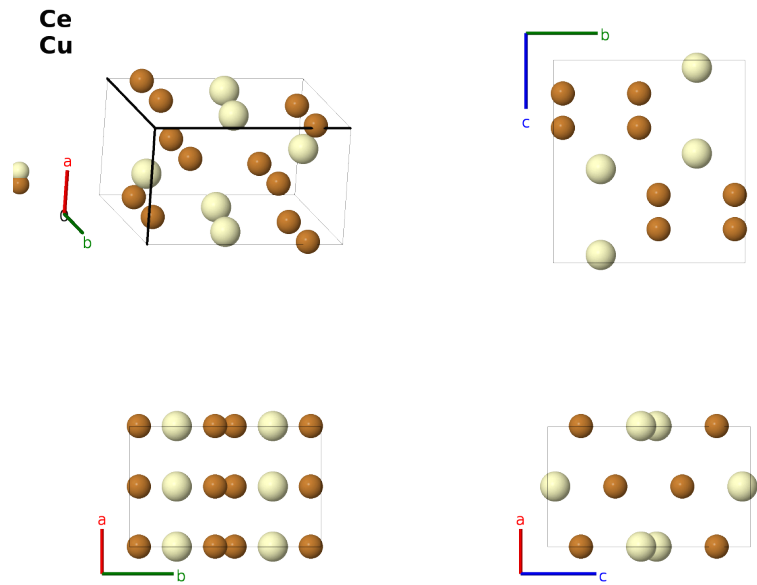
This structure previously used the label(s) **AB2_oI12_74_e_h**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/237T>

https://aflow.org/prototype-encyclopedia/AB2_oI12_74_e_h-001



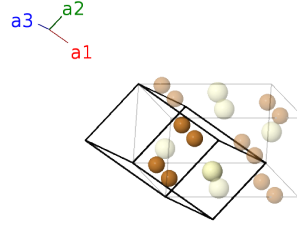
Prototype	CeCu ₂
AFLOW prototype label	AB2_oI12_74_e_h-001
ICSD	102124
CCDC	1660113
Pearson symbol	oI12
Space group number	74
Space group symbol	<i>Imma</i>
AFLOW prototype command	<code>aflow --proto=AB2_oI12_74_e_h-001</code> <code>--params=a, b/a, c/a, z₁, y₂, z₂</code>

Other compounds with this structure

CaZn₂, CeAg₂, CeAu₂, CeCu₂, CeZn₂, DyCu₂, DyZn₂, ErCu₂, ErZn₂, EuAg₂, EuAu₂, EuCu₂, EuZn₂, GdCu₂, GdZn₂, HoCu₂, HoZn₂, LaAg₂, LaAu₂, LaZn₂, LuCu₂, LuZn₂, NdAg₂, NdCu₂, NdZn₂, PrAg₂, PrCu₂, PrZn₂, SmCu₂, SmZn₂, TbCu₂, ThZn₂, TmZn₂, YbAg₂, YbCu₂, YbZn₂

Body-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \left(z_1 + \frac{1}{4}\right) \mathbf{a}_1 + z_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}b\hat{\mathbf{y}} + cz_1\hat{\mathbf{z}}$	(4e)	Ce I
$\mathbf{B}_2$	$= -\left(z_1 - \frac{3}{4}\right) \mathbf{a}_1 - z_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}b\hat{\mathbf{y}} - cz_1\hat{\mathbf{z}}$	(4e)	Ce I
$\mathbf{B}_3$	$= (y_2 + z_2) \mathbf{a}_1 + z_2 \mathbf{a}_2 + y_2 \mathbf{a}_3$	$=$	$by_2\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(8h)	Cu I
$\mathbf{B}_4$	$= \left(-y_2 + z_2 + \frac{1}{2}\right) \mathbf{a}_1 + z_2 \mathbf{a}_2 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-b\left(y_2 - \frac{1}{2}\right)\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(8h)	Cu I
$\mathbf{B}_5$	$= \left(y_2 - z_2 + \frac{1}{2}\right) \mathbf{a}_1 - z_2 \mathbf{a}_2 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}} - cz_2\hat{\mathbf{z}}$	(8h)	Cu I
$\mathbf{B}_6$	$= -(y_2 + z_2) \mathbf{a}_1 - z_2 \mathbf{a}_2 - y_2 \mathbf{a}_3$	$=$	$-by_2\hat{\mathbf{y}} - cz_2\hat{\mathbf{z}}$	(8h)	Cu I

References

- [1] A. C. Larson and D. T. Cromer, *The crystal structure of CeCu₂*, Acta Cryst. **14**, 73–74 (1961), doi:10.1107/S0365110X61000231.
- [2] D. Debray, *Crystal Chemistry of the CeCu₂-type structure*, J. Less-Common Met. **30**, 237–248 (1973), doi:10.1016/0022-5088(73)90110-0.

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