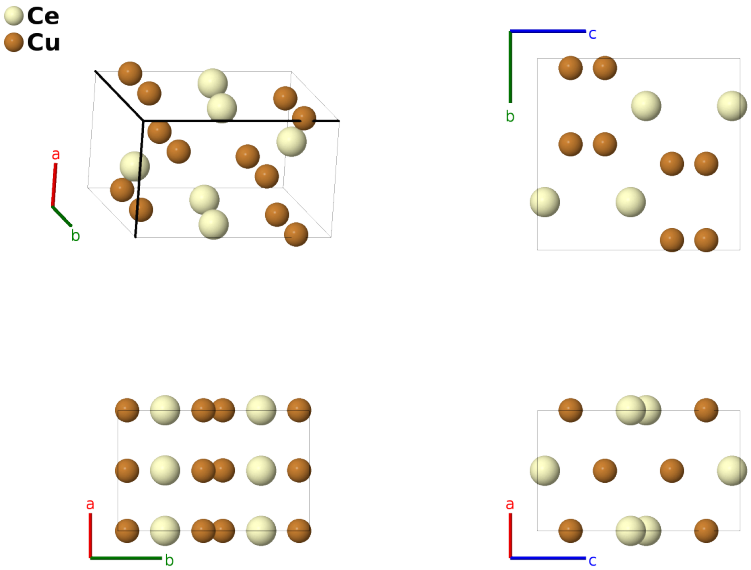
$CeCu_2$ Structure: AB2_oI12_74_e_h-001

This structure originally had the label `AB2_oI12_74_e_h`. Calls to that address will be redirected here.

Cite this page as: 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/p/237T

https://aflow.org/p/AB2_oI12_74_e_h-001



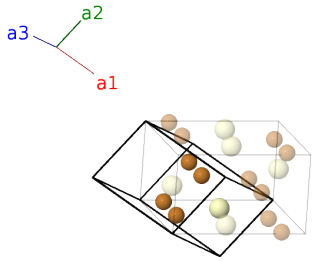
Prototype	$CeCu_2$
AFLOW prototype label	AB2_oI12_74_e_h-001
ICSD	102124
Pearson symbol	oI12
Space group number	74
Space group symbol	$Imma$
AFLOW prototype command	`aflow --proto=AB2_oI12_74_e_h-001 --params=`$a, b/a, c/a, z_1, y_2, z_2$

Other compounds with this structure

$CaZn_2$, $CeAg_2$, $CeAu_2$, $CeCu_2$, $CeZn_2$, $DyCu_2$, $DyZn_2$, $ErCu_2$, $ErZn_2$, $EuAg_2$, $EuAu_2$, $EuCu_2$, $EuZn_2$, $GdCu_2$, $GdZn_2$, $HoCu_2$, $HoZn_2$, $LaAg_2$, $LaAu_2$, $LaZn_2$, $LuCu_2$, $LuZn_2$, $NdAg_2$, $NdCu_2$, $NdZn_2$, $PrAg_2$, $PrCu_2$, $PrZn_2$, $SmCu_2$, $SmZn_2$, $TbCu_2$, $ThZn_2$, $TmZn_2$, $YbAg_2$, $YbCu_2$, $YbZn_2$

Body-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



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 $CeCu_2$*, Acta Cryst. **14**, 73–74 (1961), doi:10.1107/S0365110X61000231.

[2] D. Debray, *Crystal Chemistry of the $CeCu_2$-type structure*, J. Less-Common Met. **30**, 237–248 (1973), doi:10.1016/0022-5088(73)90110-0.