$AuBe_5$ ($C15_b$) Structure: AB5_cF24_216_a_ce-001

This structure originally had the label `AB5_cF24_216_a_ce`. Calls to that address will be redirected here.

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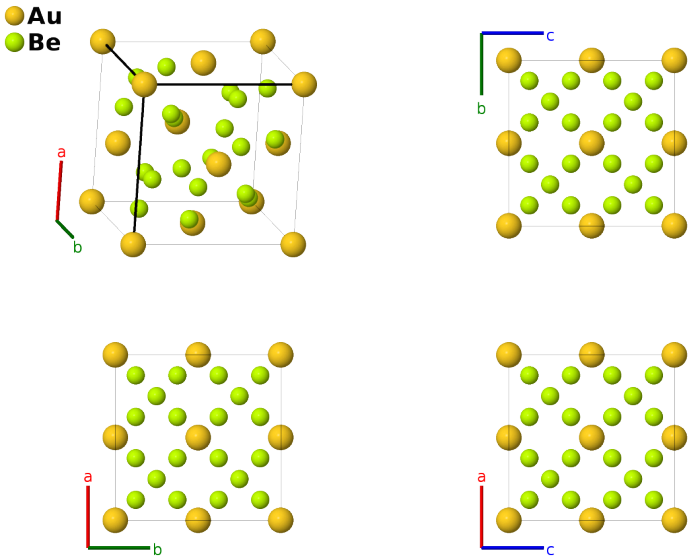
https://aflow.org/p/3454

https://aflow.org/p/AB5_cF24_216_a_ce-001



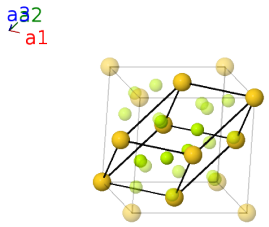
Prototype	$AuBe_5$
AFLOW prototype label	AB5_cF24_216_a_ce-001
***Strukturbericht* designation**	$C15_b$
ICSD	611643
Pearson symbol	cF24
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	`aflow --proto=AB5_cF24_216_a_ce-001 --params=`a, x_3

Other compounds with this structure
$CaAu_5$, $CoBe_5$, $HfNi_5$, $PdBe_5$, UCu_5, UNi_5, UPt_5, $ZrNi_5$, $CaNi_4Mg$, $CeNi_4Mg$, $DyNi_4Mg$, $ErNi_4Mg$, $HoNi_4Mg$, $InCu_4Mg$, $LaNi_4Mg$, $LuNi_4Mg$, $NdNi_4Mg$, $PrNi_4Mg$, $ScNi_4Mg$, $SmNi_4Mg$, $SnCu_4Mg$, $SnCu_4Mn$, $TbNi_4Mg$, $TmNi_4Mg$, YNi_4Mg, $YbNi_4Mg$

- The lattice constant for this structure is taken from (Batchelder, 1958), which does not give the internal coordinate for the (16c) site. However, (Baenziger, 1950) assumes that uranium compounds of this type have an internal parameter $x_3 \approx 5/8$. (Pearson, 1958) uses this to infer a value of $x_3 \approx 5/8$ here as well.

Face-centered Cubic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Au I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(4c)	Be I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16e)	Be II
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - 3x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16e)	Be II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 - 3x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(16e)	Be II
$\mathbf{B_6}$	=	$-3x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(16e)	Be II

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.

[2] F. W. von Batchelder and R. F. Raeuchle, *The tetragonal MBe_{12} structure of silver, palladium, platinum and gold*, Acta Cryst. **11**, 122 (1958), doi:10.1107/S0365110X58000323.

Found in

[1] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, Volume 2*, *International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 8 (Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1967).