$CeRu_2B_2$ Structure: A2BC2_oF40_22_ej_ac_fi-001

This structure originally had the label `A2BC2_oF40_22_fi_ad_gh`. Calls to that address will be redirected here.

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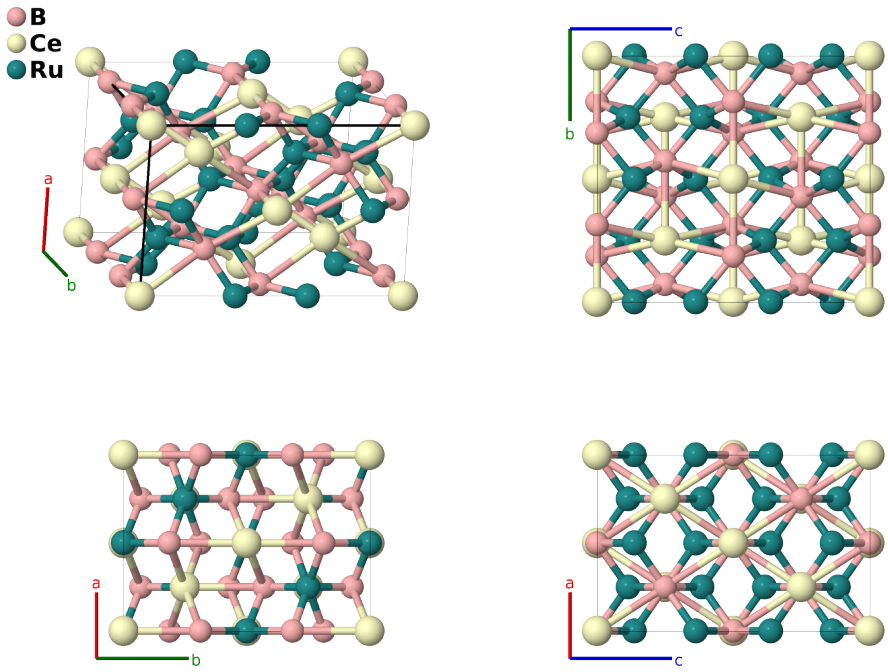
https://aflow.org/p/PN0D

https://aflow.org/p/A2BC2_oF40_22_ej_ac_fi-001



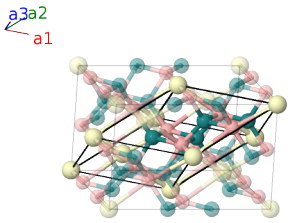
Prototype	B_2CeRu_2
AFLOW prototype label	A2BC2_oF40_22_ej_ac_fi-001
ICSD	40800
Pearson symbol	oF40
Space group number	22
Space group symbol	$F222$
AFLOW prototype command	`aflow --proto=A2BC2_oF40_22_ej_ac_fi-001 --params=`$a, b/a, c/a, x_3, y_4, y_5, x_6$

Other compounds with this structure
$CeOs_2B_2$, $GdOs_2B_2$, $GdRu_2B_2$, $LaOs_2B_2$, $LaRu_2B_2$, $NdOs_2B_2$, $NdRu_2B_2$, $PrOs_2B_2$, $PrRu_2B_2$, $SmOs_2B_2$, $SmRu_2B_2$, $ThOs_2B_2$, $ThRu_2B_2$

- As noted by (Horvath, 1987) a small amount of uncertainty in the positions of the atoms would allow this system to be placed in the centrosymmetric space group $Fddd$ #70.

Face-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Ce I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Ce II
$\mathbf{B_3}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(8e)	B I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(8e)	B I
$\mathbf{B_5}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}}$	(8f)	Ru I
$\mathbf{B_6}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}}$	(8f)	Ru I
$\mathbf{B_7}$	=	$y_5\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + y_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8i)	Ru II
$\mathbf{B_8}$	=	$-\left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8i)	Ru II
$\mathbf{B_9}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8j)	B II
$\mathbf{B_{10}}$	=	$x_6\,\mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8j)	B II

References

[1] C. Horvath, P. Rogle, and K. Hiebl, *The crystal structure of $CeRu_2B_2$ and isotypic compounds $M(Ru, Os)_2B_2$, M = La, Pr, Nd, Sm, Gd, and Th*, J. Solid State Chem. **67**, 70–77 (1987), doi:10.1016/0022-4596(87)90340-9.