# $CeRu_2B_2$ Structure: A2BC2_oF40_22_ej_ac_fi-001

This structure previously used the label(s) `A2BC2_oF40_22_fi_ad_gh`. Calls to these addresses will be redirected here.

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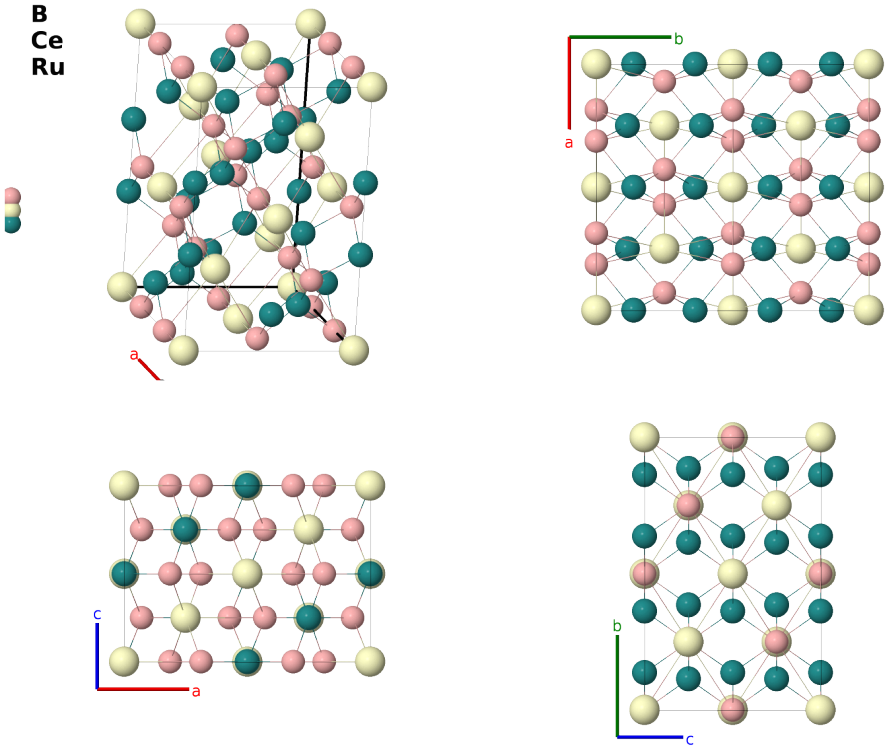
https://aflow.org/prototype-encyclopedia/PN0D

https://aflow.org/prototype-encyclopedia/A2BC2_oF40_22_ej_ac_fi-001



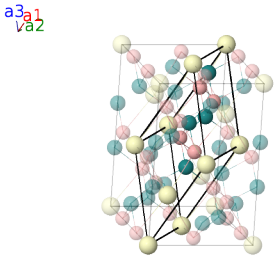

| | |
|---|---|
| **Prototype** | $B_2CeRu_2$ |
| **AFLOW prototype label** | A2BC2_oF40_22_ej_ac_fi-001 |
| **ICSD** | 40800 |
| **CCDC** | 161062 |
| **Pearson symbol** | oF40 |
| **Space group number** | 22 |
| **Space group symbol** | $F222$ |
| **AFLOW prototype command** | `aflow --proto=A2BC2_oF40_22_ej_ac_fi-001 --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**

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




**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.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