# $Ba_xPt_3B_2$ Structure: A2BC3_hP12_194_f_a_h-001

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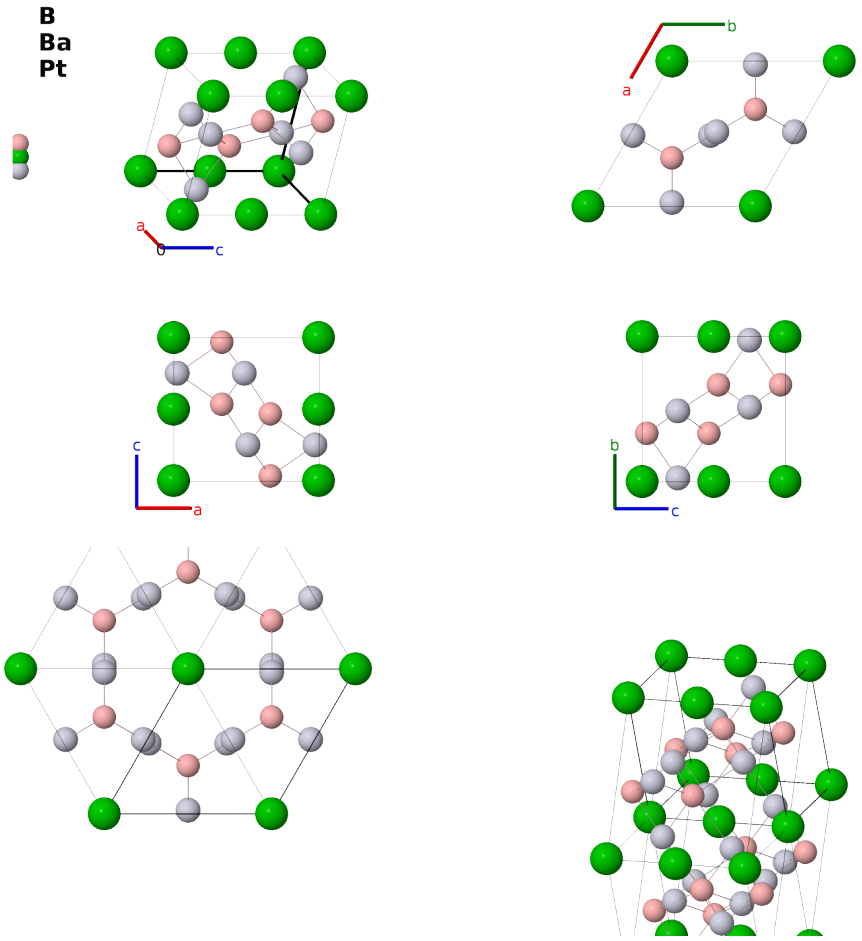
https://aflow.org/prototype-encyclopedia/UW0R

https://aflow.org/prototype-encyclopedia/A2BC3_hP12_194_f_a_h-001




| | |
|---|---|
| **Prototype** | $B_2BaPt_3$ |
| **AFLOW prototype label** | A2BC3_hP12_194_f_a_h-001 |
| **ICSD** | 43994 |
| **CCDC** | 1613435 |
| **Pearson symbol** | hP12 |
| **Space group number** | 194 |
| **Space group symbol** | $P6_3/mmc$ |

**AFLOW prototype command** `aflow --proto=A2BC3_hP12_194_f_a_h-001 --params=`$a, c/a, z_2, x_3$

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**Other compounds with this structure**

$Ca_xPt_3B_2$, $Sr_xPt_3B_2$

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- These are all superconducting structures with $T_c$ in the range 1.6-5.5 K.
- The (2a) site is approximately 2/3 occupied in all of these materials.
- (Shelton, 1978) did not specify the value of $z_2$. We infer a value of 0.03265 from the minimum B-B distance of 2.29Å given in the paper.
- $U_2Cr_3Si$, AFLOW label A3BC2_hP12_194_h_a_f-002, and $Ba_xPt_3B_2$, A2BC3_hP12_194_f_a_h, occupy the same Wyckoff positions in space group $P6_3/mmc$ # 194. They differ in the c/a ratio, with $U_2Cr_3Si$ having $c/a \approx 1.6$ and $Ba_xPt_3B_2$ $c/a \approx 0.85$.

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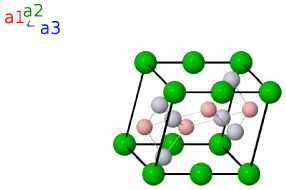
**Hexagonal primitive vectors**

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (2a) | Ba I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}c\,\hat{\mathbf{z}}$ | (2a) | Ba I |
| $\mathbf{B_3}$ | = | $\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (4f) | B I |
| $\mathbf{B_4}$ | = | $\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (4f) | B I |
| $\mathbf{B_5}$ | = | $\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$ | (4f) | B I |
| $\mathbf{B_6}$ | = | $\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (4f) | B I |
| $\mathbf{B_7}$ | = | $x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (6h) | Pt I |
| $\mathbf{B_8}$ | = | $-2x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $-\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (6h) | Pt I |
| $\mathbf{B_9}$ | = | $x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $-\sqrt{3}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (6h) | Pt I |
| $\mathbf{B_{10}}$ | = | $-x_3\,\mathbf{a}_1 - 2x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $-\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (6h) | Pt I |
| $\mathbf{B_{11}}$ | = | $2x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (6h) | Pt I |
| $\mathbf{B_{12}}$ | = | $-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $\sqrt{3}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (6h) | Pt I |

**References**


[1] R. N. Shelton, *Superconductivity and crystal structure of a new class of ternary platinum borides*, J. Less-Common Met. **62**, 191–196 (1978), doi:10.1016/0022-5088(78)90031-0.

**Found in**

[1] *Inorganic Crystal Structure Database*. Entry 83037 [BaPt3B2].

**First cited in**

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