

ZrBr Structure:

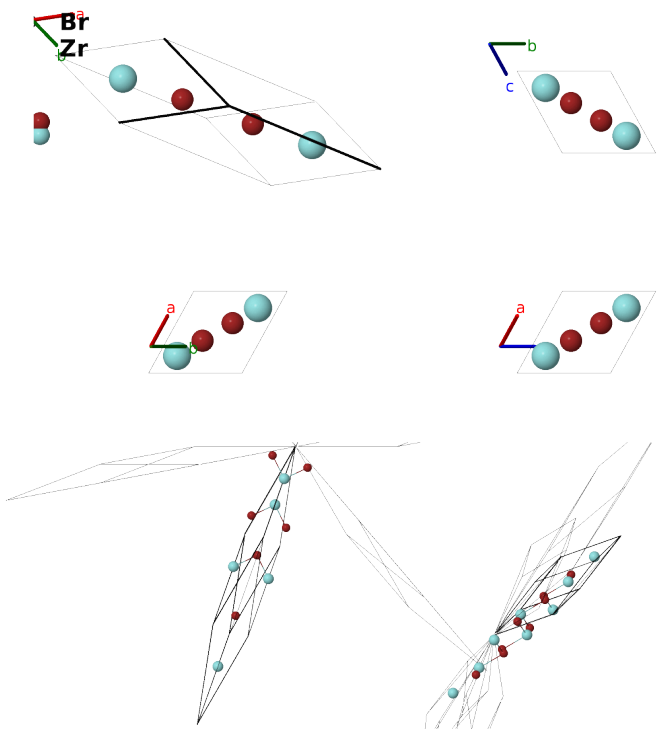
AB_hR4_166_c_c-006

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/prototype-encyclopedia/C7FB>

https://aflow.org/prototype-encyclopedia/AB_hR4_166_c_c-006



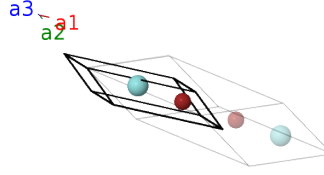
Prototype	BrZr
AFLOW prototype label	AB_hR4_166_c_c-006
ICSD	1168
CCDC	1591348
Pearson symbol	hR4
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=AB_hR4_166_c_c-006</code> <code>--params=$a, c/a, x_1, x_2$</code>

Other compounds with this structure
HfCl, ScCl

- Rhombohedral ZrCl and ZrBr have the same AFLOW prototype label, AB_hR4_166_c_c, and the ICSD lists both structures under structure type ZrCl.
- However, the stacking order and the intra-layer atom distance is substantially different in the two systems, so we separate them.
- The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Rhombohedral primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{1}{3}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a\hat{\mathbf{y}} + \frac{1}{3}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{1}{3}c\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$cx_1 \hat{\mathbf{z}}$	(2c)	Br I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-cx_1 \hat{\mathbf{z}}$	(2c)	Br I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(2c)	Zr I
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-cx_2 \hat{\mathbf{z}}$	(2c)	Zr I

References

- [1] R. L. Daake and J. D. Corbett, *Zirconium monobromide, a second double metal sheet structure. Some physical and chemical properties of the metallic zirconium monochloride and monobromide*, Inorg. Chem. **16**, 2029–2033 (1977), doi:10.1021/ic50174a041.

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