Rhombohedral ZrCl Structure: AB_hR4_166_c_c-005

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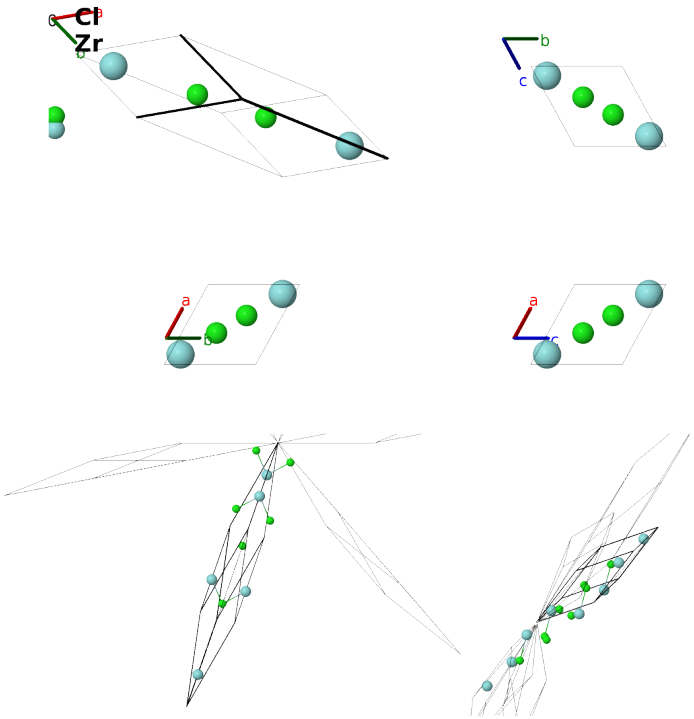
https://aflow.org/prototype-encyclopedia/7TJQ

https://aflow.org/prototype-encyclopedia/AB_hR4_166_c_c-005



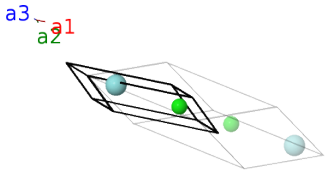
Prototype	ClZr
AFLOW prototype label	AB_hR4_166_c_c-005
ICSD	869
CCDC	1591113
Pearson symbol	hR4
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=AB_hR4_166_c_c-005 --params=`$a, c/a, x_1, x_2$

- ZrCl can also be found in a monoclinic structure.
- 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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



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)	Cl 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)	Cl 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] D. G. Adolphson and J. D. Corbett, *Crystal structure of zirconium monochloride. A novel phase containing metal-metal bonded sheets*, Inorg. Chem. **15**, 1820–1823 (1976), doi:10.1021/ic50162a017.

Found in

[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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