Monoclinic ZrCl Structure: AB_mC8_12_i_i-002

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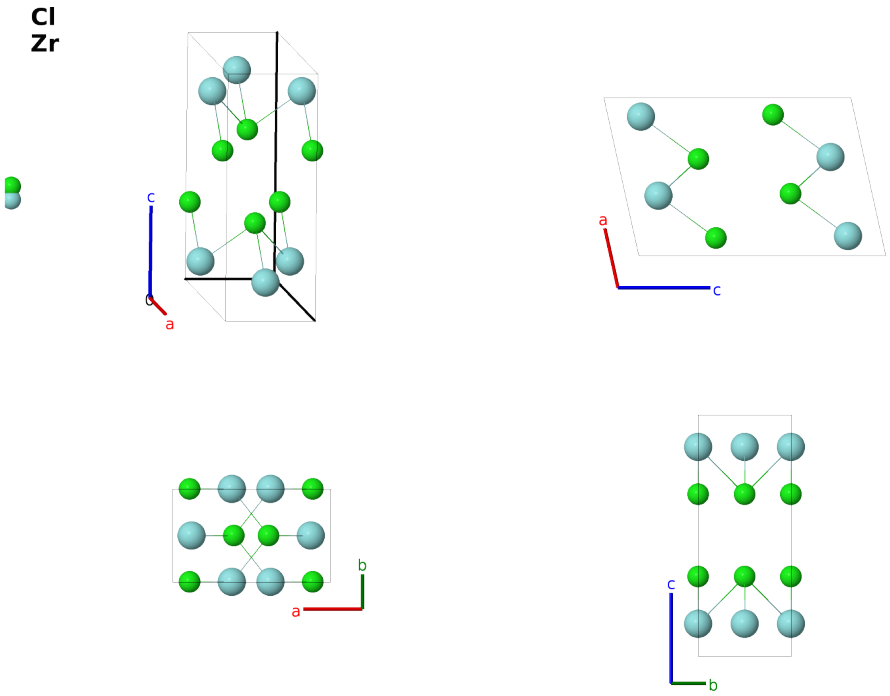
https://aflow.org/prototype-encyclopedia/S8YA

https://aflow.org/prototype-encyclopedia/AB_mC8_12_i_i-002



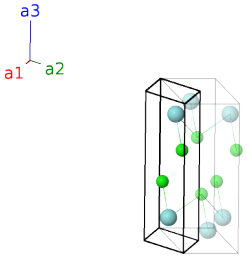
Prototype	ClZr
AFLOW prototype label	AB_mC8_12_i_i-002
ICSD	868
CCDC	1591112
Pearson symbol	mC8
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=AB_mC8_12_i_i-002 --params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2$

- (Adolphson, 1976) put ZrCl in space group $C2$ #5, but since the set the y-coordinates of both atoms to zero there is an inversion site and the space group becomes $C2/m$ #12.

- ZrCl can also be found in a rhombohedral structure.

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(4i)	Cl I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(4i)	Cl I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Zr I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	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

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