Cs_3CoCl_5 ($K3_1$) Structure: A5BC3_tI36_140_cl_b_ah-001

This structure previously used the label(s) `A5BC3_tI36_140_cl_b_ah`. Calls to these addresses will be redirected here.

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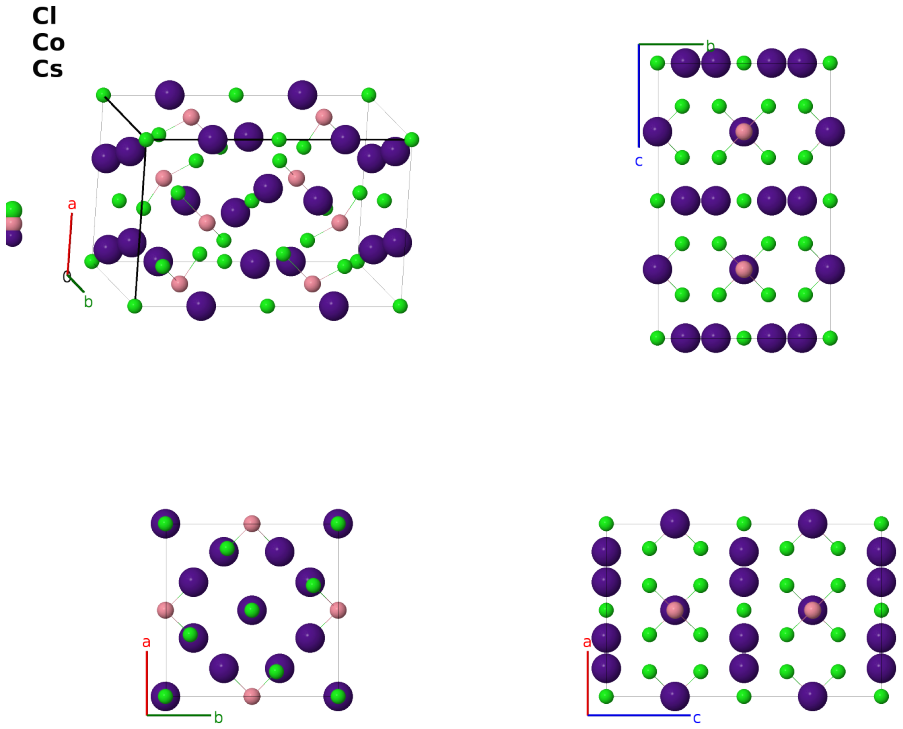
https://aflow.org/prototype-encyclopedia/GHEH

https://aflow.org/prototype-encyclopedia/A5BC3_tI36_140_cl_b_ah-001



Prototype	Cl_5CoCs_3
AFLOW prototype label	A5BC3_tI36_140_cl_b_ah-001
***Strukturbericht* designation**	$K3_1$
ICSD	14087
CCDC	1595491
Pearson symbol	tI36
Space group number	140
Space group symbol	$I4/mcm$

AFLOW prototype command `aflow --proto=A5BC3_tI36_140_cl_b_ah-001 --params=`$a, c/a, x_4, x_5, z_5$

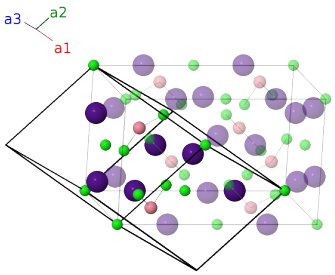
Other compounds with this structure

Ba_3CrO_5, Ba_3SiO_5, Ba_3TiS_5, Cl_3OLi_5, Cs_3CdBr_5, Cs_3CdD_5, Cs_3CoBr_5, Cs_3CoCl_5, Cs_3FeBr_5, Cs_3FeCl_5, Cs_3MgD_5, Cs_3MnBr_5, Cs_3MnD_5, Cs_3MnI_5, Cs_3NiCl_5, Cs_3ZnBr_5, Cs_3ZnCl_5, Cs_3ZnH_5, Eu_3AlO_5, K_3MnH_5, K_3ZnH_5, La_3CrN_5, La_3MnN_5, La_3MoN_5, Pb_3OCe_5, Pb_3OLa_5, Rb_3CoBr_5, Rb_3MgD_5, Rb_3MnD_5, Rb_3ZnH_5, Sr_3CO_5, Tl_3CoCl_5, Tl_3FeCl_5, Cs_3CoBr_5, Cs_3ZnH_5, Rb_3ZnH_5, Ba_3MO_5, (M = tetravalent metal), $CsBa_5Ti_2Se_9Cl$, $(Sr_{3-x}A_x)AlO_4F$, (A = Ba, Ca), $M_3Mg(BH_4)_5$, (M = Rb, Cs)

- We show the structure using the data taken at 4.2K.
- We list the quaternary form of this structure as $BaLa_2ZnO_5$.
- Removing the Cl-II atoms from the (4c) site reduces this to the $NH_4Pb_2Br_5$ ($K3_4$) structure.
- There are many quaternary compounds with this structure. See the $BaLa_2ZnO_5$ prototype for more details.
- We assign compounds with different species on the (4a) and (16l) Wyckoff sites to the K_2BaPO_4F structure prototype. The ICSD lists all of these prototypes under the Cs_3CoCl_5 structure type.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	Cs I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	Cs I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	Co I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	Co I
$\mathbf{B_5}$	=	0	=	0	(4c)	Cl I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	Cl I
$\mathbf{B_7}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(2x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	Cs II
$\mathbf{B_8}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - \left(2x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	Cs II
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(8h)	Cs II
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(8h)	Cs II
$\mathbf{B_{11}}$	=	$\left(x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + \left(2x_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16l)	Cl II

$\mathbf{B_{12}}$	$=$	$\left(-x_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_5-z_5\right)\,\mathbf{a}_2-\left(2x_5-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(16l)	Cl II
$\mathbf{B_{13}}$	$=$	$\left(x_5+z_5\right)\,\mathbf{a}_1+\left(-x_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(16l)	Cl II
$\mathbf{B_{14}}$	$=$	$-\left(x_5-z_5\right)\,\mathbf{a}_1+\left(x_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(16l)	Cl II
$\mathbf{B_{15}}$	$=$	$\left(x_5-z_5\right)\,\mathbf{a}_1-\left(x_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(16l)	Cl II
$\mathbf{B_{16}}$	$=$	$-\left(x_5+z_5\right)\,\mathbf{a}_1+\left(x_5-z_5+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(16l)	Cl II
$\mathbf{B_{17}}$	$=$	$\left(x_5-z_5+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_5-z_5\right)\,\mathbf{a}_2+\left(2x_5+\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$ax_5\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(16l)	Cl II
$\mathbf{B_{18}}$	$=$	$-\left(x_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_5+z_5\right)\,\mathbf{a}_2-\left(2x_5-\frac{1}{2}\right)\,\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(16l)	Cl II

References

[1] B. N. Figgis, R. Mason, A. R. P. Smith, and G. A. Williams, *Neutron Diffraction Structure of Cs_3CoCl_5 at 4.2K*, Acta Crystallogr. Sect. B **36**, 509–512 (1980), doi:10.1107/S0567740880003731.

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