$Cs_3Tl_2Cl_9$ ($K7_2$) Structure: A9B3C2_hR28_167_ef_e_c-001

This structure originally had the label `A9B3C2_hR28_167_ef_e_c`. Calls to that address will be redirected here.

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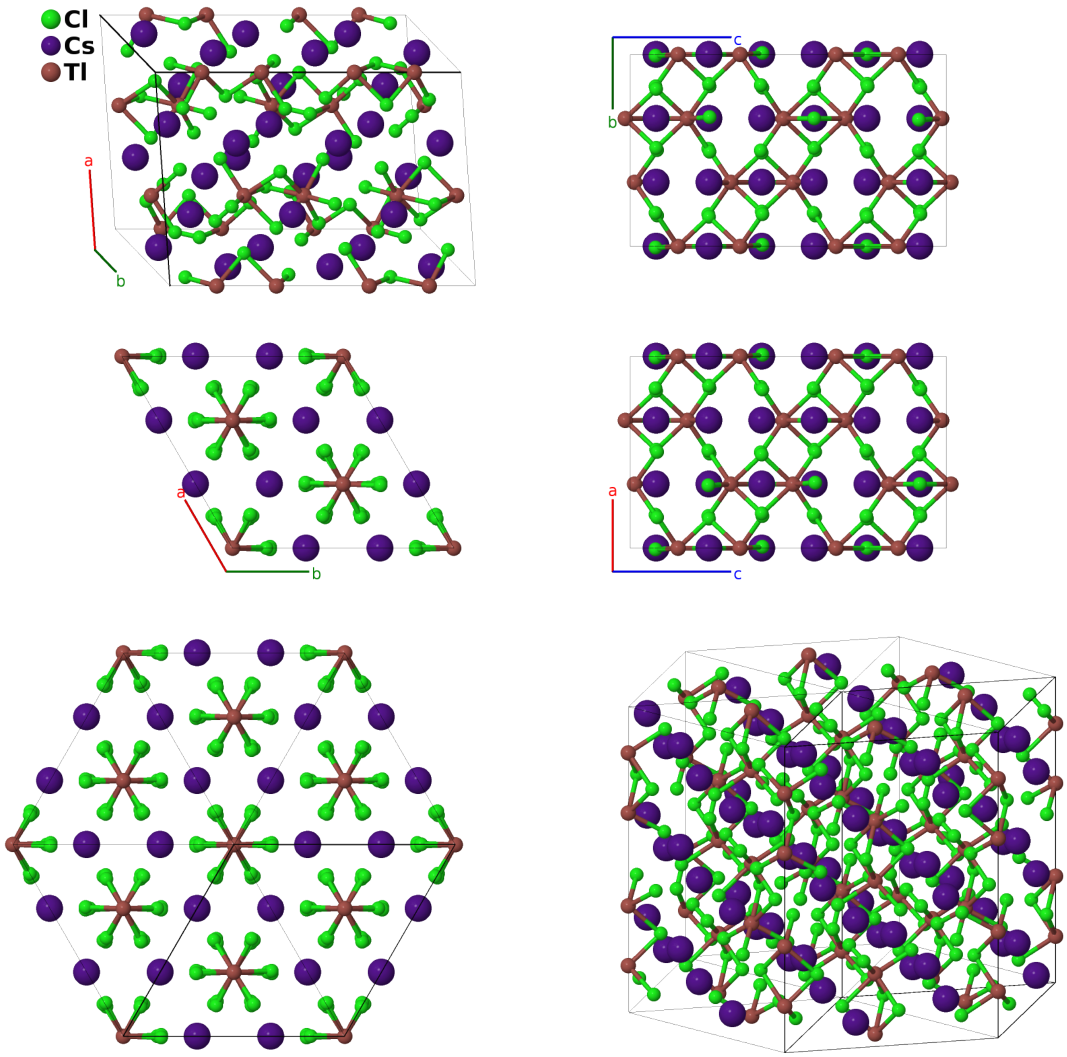
https://aflow.org/p/7M03

https://aflow.org/p/A9B3C2_hR28_167_ef_e_c-001



Prototype	$Cl_9Cs_3Tl_2$
AFLOW prototype label	A9B3C2_hR28_167_ef_e_c-001
***Strukturbericht* designation**	$K7_2$
ICSD	27849
Pearson symbol	hR28
Space group number	167

Space group symbol $R\bar{3}c$

AFLOW prototype command `aflow --proto=A9B3C2_hR28_167_ef_e_c-001`
`--params=`$a, c/a, x_1, x_2, x_3, x_4, y_4, z_4$

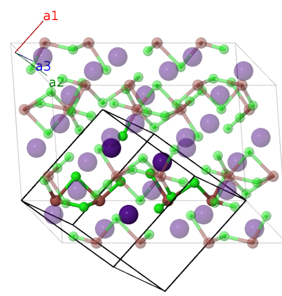
Other compounds with this structure

$Cs_3Dy_2Br_9$, $Cs_3Er_2Br_9$, $Cs_3Ho_2Br_9$, $Cs_3Lu_2Cl_9$, $Cs_3Tb_2Br_9$, $Cs_3Yb_2Br_9$, $Ba_3Os_2O_9$, $Ba_3W_2O_9$

- (Hoard, 1935) followed by (Downs, 2003), give the atomic coordinates in the style of (Wyckoff, 1922), who lists space group D_{3d}^6 (the Schönflies notation for space group $R\bar{3}c$) as space group #203, instead of #167, and uses an origin which corresponds to (1/4 1/4 1/4) in our lattice coordinates. We used FINDSYM to convert this into our standard setting for space group #167.

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a_1} + x_1\,\mathbf{a_2} + x_1\,\mathbf{a_3}$	=	$cx_1\,\hat{\mathbf{z}}$	(4c)	Tl I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\mathbf{a_1} - \left(x_1 - \frac{1}{2}\right)\mathbf{a_2} - \left(x_1 - \frac{1}{2}\right)\mathbf{a_3}$	=	$-c\left(x_1 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Tl I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a_1} - x_1\,\mathbf{a_2} - x_1\,\mathbf{a_3}$	=	$-cx_1\,\hat{\mathbf{z}}$	(4c)	Tl I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\mathbf{a_1} + \left(x_1 + \frac{1}{2}\right)\mathbf{a_2} + \left(x_1 + \frac{1}{2}\right)\mathbf{a_3}$	=	$c\left(x_1 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(4c)	Tl I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a_1} - \left(x_2 - \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$	=	$\frac{1}{8}a\left(4x_2 - 1\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a\left(4x_2 - 1\right)\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	Cl I
$\mathbf{B_6}$	=	$\frac{1}{4}\,\mathbf{a_1} + x_2\,\mathbf{a_2} - \left(x_2 - \frac{1}{2}\right)\mathbf{a_3}$	=	$\frac{1}{8}a\left(4x_2 - 1\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a\left(4x_2 - 1\right)\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	Cl I
$\mathbf{B_7}$	=	$-\left(x_2 - \frac{1}{2}\right)\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} + x_2\,\mathbf{a_3}$	=	$-a\left(x_2 - \frac{1}{4}\right)\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	Cl I
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a_1} + \left(x_2 + \frac{1}{2}\right)\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$	=	$-\frac{1}{8}a\left(4x_2 + 3\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a\left(12x_2 + 1\right)\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	Cl I
$\mathbf{B_9}$	=	$\frac{3}{4}\,\mathbf{a_1} - x_2\,\mathbf{a_2} + \left(x_2 + \frac{1}{2}\right)\mathbf{a_3}$	=	$-\frac{1}{8}a\left(4x_2 - 1\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a\left(12x_2 + 5\right)\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	Cl I
$\mathbf{B_{10}}$	=	$\left(x_2 + \frac{1}{2}\right)\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} - x_2\,\mathbf{a_3}$	=	$a\left(x_2 + \frac{1}{4}\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	Cl I
$\mathbf{B_{11}}$	=	$x_3\,\mathbf{a_1} - \left(x_3 - \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$	=	$\frac{1}{8}a\left(4x_3 - 1\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a\left(4x_3 - 1\right)\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	Cs I
$\mathbf{B_{12}}$	=	$\frac{1}{4}\,\mathbf{a_1} + x_3\,\mathbf{a_2} - \left(x_3 - \frac{1}{2}\right)\mathbf{a_3}$	=	$\frac{1}{8}a\left(4x_3 - 1\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a\left(4x_3 - 1\right)\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	Cs I
$\mathbf{B_{13}}$	=	$-\left(x_3 - \frac{1}{2}\right)\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} + x_3\,\mathbf{a_3}$	=	$-a\left(x_3 - \frac{1}{4}\right)\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	Cs I
$\mathbf{B_{14}}$	=	$-x_3\,\mathbf{a_1} + \left(x_3 + \frac{1}{2}\right)\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$	=	$-\frac{1}{8}a\left(4x_3 + 3\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a\left(12x_3 + 1\right)\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	Cs I
$\mathbf{B_{15}}$	=	$\frac{3}{4}\,\mathbf{a_1} - x_3\,\mathbf{a_2} + \left(x_3 + \frac{1}{2}\right)\mathbf{a_3}$	=	$-\frac{1}{8}a\left(4x_3 - 1\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a\left(12x_3 + 5\right)\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	Cs I
$\mathbf{B_{16}}$	=	$\left(x_3 + \frac{1}{2}\right)\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} - x_3\,\mathbf{a_3}$	=	$a\left(x_3 + \frac{1}{4}\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	Cs I
$\mathbf{B_{17}}$	=	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	=	$\frac{1}{2}a\left(x_4 - z_4\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_4 - 2y_4 + z_4\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}}$	(12f)	Cl II
$\mathbf{B_{18}}$	=	$z_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + y_4\,\mathbf{a_3}$	=	$-\frac{1}{2}a\left(y_4 - z_4\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_4 - y_4 - z_4\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_4 + y_4 + z_4\right)\hat{\mathbf{z}}$	(12f)	Cl II

$\mathbf{B_{19}}$	=	$y_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(12f)	Cl II
$\mathbf{B_{20}}$	=	$-\left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_4 - 2y_4 + z_4)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_4 + 2y_4 + 2z_4 - 3)\,\hat{\mathbf{z}}$	(12f)	Cl II
$\mathbf{B_{21}}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_4 - z_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_4 - y_4 - z_4)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_4 + 2y_4 + 2z_4 - 3)\,\hat{\mathbf{z}}$	(12f)	Cl II
$\mathbf{B_{22}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 - y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(2x_4 + 2y_4 + 2z_4 - 3)\,\hat{\mathbf{z}}$	(12f)	Cl II
$\mathbf{B_{23}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_4 - 2y_4 + z_4)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(12f)	Cl II
$\mathbf{B_{24}}$	=	$-z_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_4 - z_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_4 - y_4 - z_4)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(12f)	Cl II
$\mathbf{B_{25}}$	=	$-y_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_4 + y_4 + z_4)\,\hat{\mathbf{z}}$	(12f)	Cl II
$\mathbf{B_{26}}$	=	$\left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_4 - z_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_4 - 2y_4 + z_4)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_4 + 2y_4 + 2z_4 + 3)\,\hat{\mathbf{z}}$	(12f)	Cl II
$\mathbf{B_{27}}$	=	$\left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_4 - z_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_4 - y_4 - z_4)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_4 + 2y_4 + 2z_4 + 3)\,\hat{\mathbf{z}}$	(12f)	Cl II
$\mathbf{B_{28}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_4 + y_4 - 2z_4)\,\hat{\mathbf{y}} + \frac{1}{6}c\,(2x_4 + 2y_4 + 2z_4 + 3)\,\hat{\mathbf{z}}$	(12f)	Cl II

References

[1] J. L. Hoard and L. Goldstein, *The Crystal Structure of Cesium Enneachlordithalliate, $Cs_3Tl_2Cl_9$*, J. Chem. Phys. **3**, 199–202 (1935), doi:10.1063/1.1749633.

[2] R. W. G. Wyckoff, *The Analytical Expression of the Results of the Theory of Space-Groups*, vol. 318 (Carnegie Institution of Washington, Washington DC, 1922).

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).