

Cs₃As₂Cl₉ (*K7*₃) Structure: A2B9C3_hP14_150_d_eg_ad-001

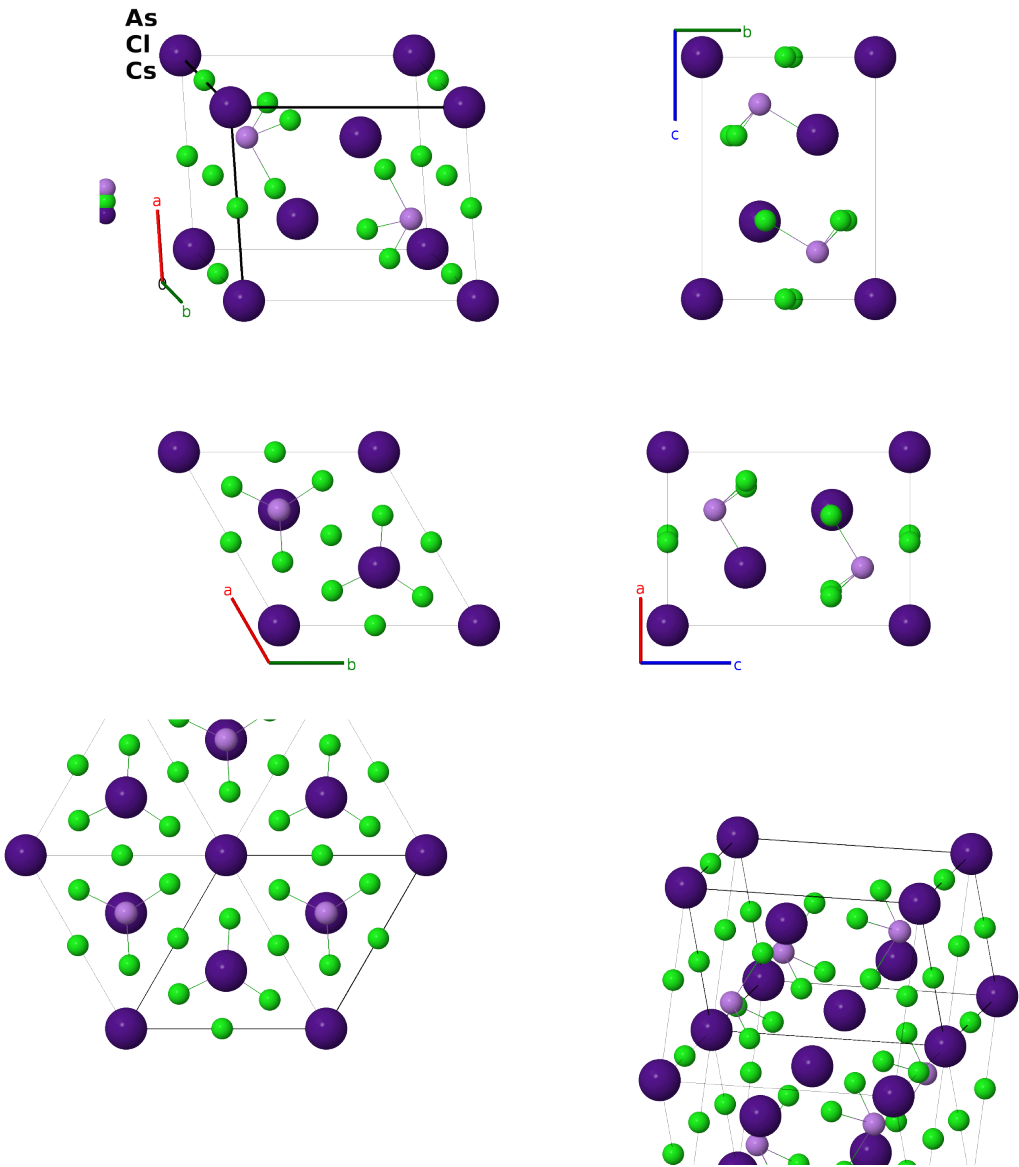
This structure previously used the label(s) **A2B9C3_hP14_150_d_eg_ad**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, 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/4FK1>

https://aflow.org/prototype-encyclopedia/A2B9C3_hP14_150_d_eg_ad-001



Prototype

As₂Cl₉Cs₃

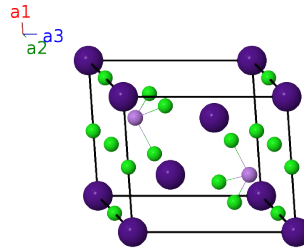
AFLOW prototype label

A2B9C3_hP14_150_d_eg_ad-001

<i>Strukturbericht</i> designation	$K7_3$
ICSD	45733
CCDC	1614356
Pearson symbol	hP14
Space group number	150
Space group symbol	$P321$
AFLOW prototype command	<code>aflow --proto=A2B9C3_hP14_150_d_eg_ad-001</code> <code>--params=a, c/a, z₂, z₃, x₄, x₅, y₅, z₅</code>

Trigonal (Hexagonal) primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(1a) Cs I
$\mathbf{B}_2$	$=$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + z_2\mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2d) As I
$\mathbf{B}_3$	$=$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 - z_2\mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(2d) As I
$\mathbf{B}_4$	$=$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + z_3\mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2d) Cs II
$\mathbf{B}_5$	$=$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 - z_3\mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(2d) Cs II
$\mathbf{B}_6$	$=$	$x_4\mathbf{a}_1$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}}$	(3e) Cl I
$\mathbf{B}_7$	$=$	$x_4\mathbf{a}_2$	$=$	$\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}}$	(3e) Cl I
$\mathbf{B}_8$	$=$	$-x_4\mathbf{a}_1 - x_4\mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}}$	(3e) Cl I
$\mathbf{B}_9$	$=$	$x_5\mathbf{a}_1 + y_5\mathbf{a}_2 + z_5\mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6g) Cl II
$\mathbf{B}_{10}$	$=$	$-y_5\mathbf{a}_1 + (x_5 - y_5)\mathbf{a}_2 + z_5\mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6g) Cl II
$\mathbf{B}_{11}$	$=$	$-(x_5 - y_5)\mathbf{a}_1 - x_5\mathbf{a}_2 + z_5\mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(6g) Cl II
$\mathbf{B}_{12}$	$=$	$y_5\mathbf{a}_1 + x_5\mathbf{a}_2 - z_5\mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(6g) Cl II
$\mathbf{B}_{13}$	$=$	$(x_5 - y_5)\mathbf{a}_1 - y_5\mathbf{a}_2 - z_5\mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(6g) Cl II
$\mathbf{B}_{14}$	$=$	$-x_5\mathbf{a}_1 - (x_5 - y_5)\mathbf{a}_2 - z_5\mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(6g) Cl II

References

- [1] J. L. Hoard and L. Goldstein, *The Structure of Caesium Enneachlordiarsenite, $Cs_3As_2Cl_9$* , J. Chem. Phys. **3**, 117–122 (1935), doi:10.1063/1.1749606.

First cited in

D. Hicks, M. J. Mehl, M. Esters, C. Oses, 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.