

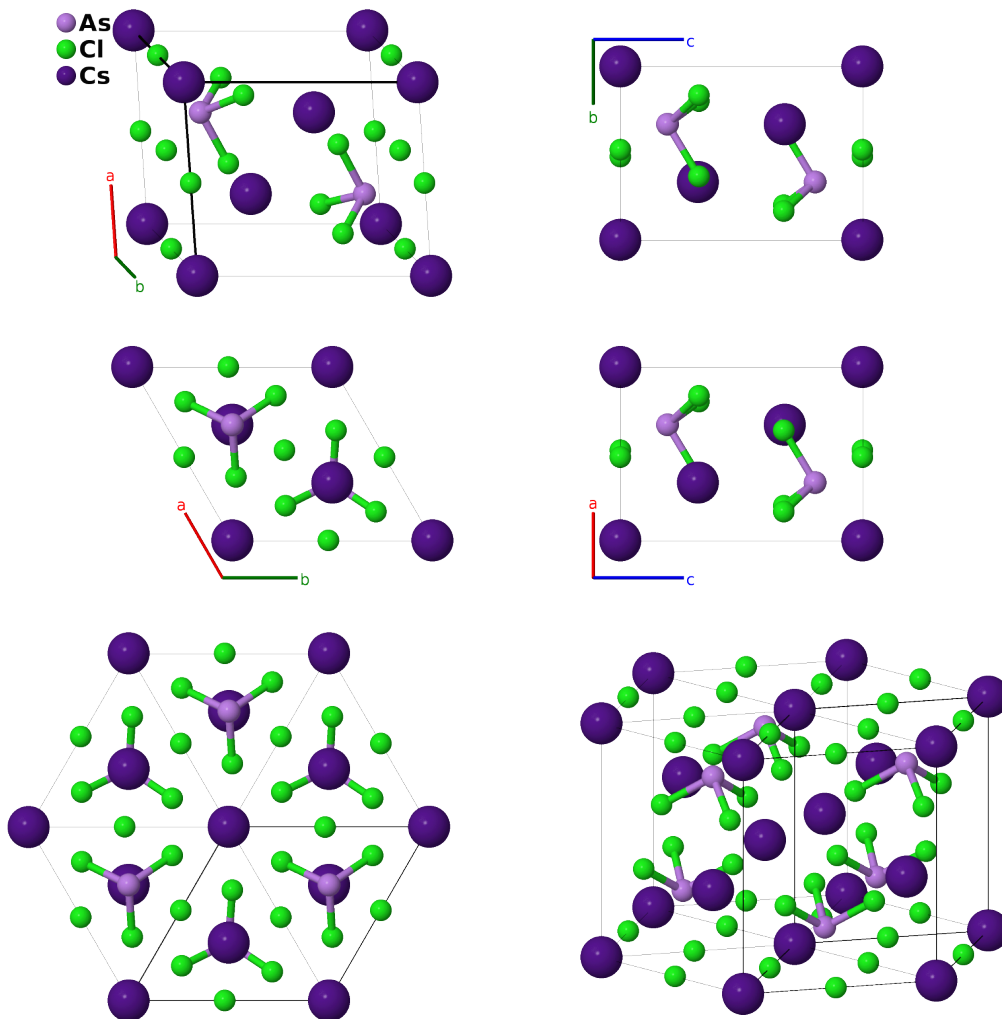
Cs₃As₂Cl₉ (*K7*₃) Structure: A2B9C3_hP14_150_d_eg_ad-001

This structure originally had the label A2B9C3_hP14_150_d_eg_ad. Calls to that address will be redirected here.

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<https://afLOW.org/p/4FK1>

https://afLOW.org/p/A2B9C3_hP14_150_d_eg_ad-001



Prototype	As ₂ Cl ₉ Cs ₃
AFLOW prototype label	A2B9C3_hP14_150_d_eg_ad-001
<i>Strukturbericht</i> designation	<i>K7</i> ₃
ICSD	45733
Pearson symbol	hP14
Space group number	150

Space group symbol

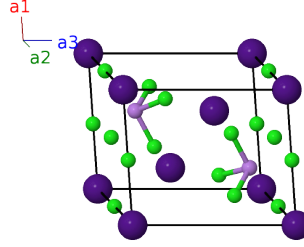
P321

AFLOW prototype command

aflow --proto=A2B9C3_hP14_150_d_eg_ad-001
 --params=a, c/a, z₂, z₃, x₄, x₅, y₅, z₅

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, Cs₃As₂Cl₉*, J. Chem. Phys. **3**, 117–122 (1935), doi:10.1063/1.1749606.