

CsC₈ Structure:

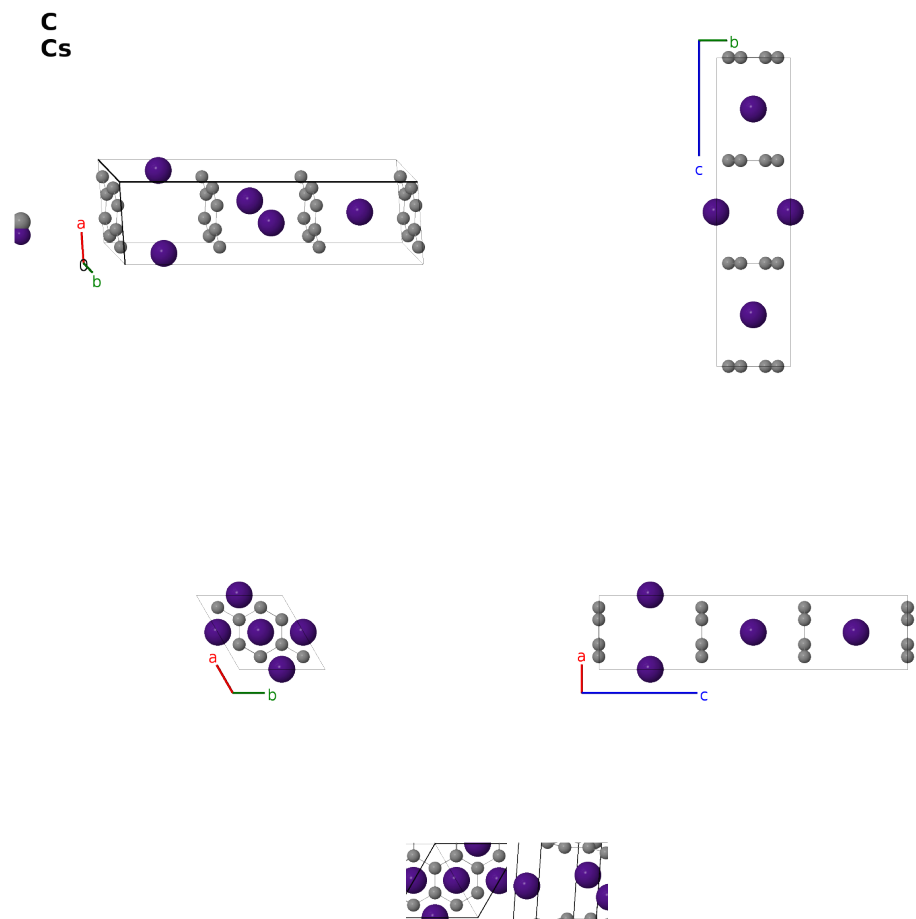
A8B_hP27_180_2ik_d-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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/T338>

https://aflow.org/prototype-encyclopedia/A8B_hP27_180_2ik_d-001

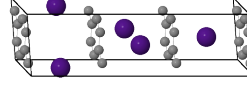


Prototype	C ₈ Cs
AFLOW prototype label	A8B_hP27_180_2ik_d-001
Pearson symbol	hP27
Space group number	180
Space group symbol	P6 ₂ 22
AFLOW prototype command	<code>aflow --proto=A8B_hP27_180_2ik_d-001</code> <code>--params=a, c/a, x₂, x₃, x₄, y₄, z₄</code>

- This is the ambient pressure structure of CsC₈. Above 1.2 GPa it transforms into an orthorhombic structure which was not determined by (Rey, 2008). Further transitions occur at higher temperatures.
- This compound can also be found in the enantiomorphic space group $P6_422$ #181. To make this transition, reflect the structure through the $z = 0$ plane.
- We found no entry in the ICSD or the CCDC for this structure.

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
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3d)	Cs I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{6} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3d)	Cs I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{5}{6} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{5}{6}c \hat{\mathbf{z}}$	(3d)	Cs I
$\mathbf{B}_4$	$= x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2$	$=$	$\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}}$	(6i)	C I
$\mathbf{B}_5$	$= -2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(6i)	C I
$\mathbf{B}_6$	$= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_2 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(6i)	C I
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 - 2x_2 \mathbf{a}_2$	$=$	$-\frac{3}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}}$	(6i)	C I
$\mathbf{B}_8$	$= 2x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(6i)	C I
$\mathbf{B}_9$	$= -x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	$=$	$\sqrt{3}ax_2 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(6i)	C I
$\mathbf{B}_{10}$	$= x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2$	$=$	$\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}}$	(6i)	C II
$\mathbf{B}_{11}$	$= -2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(6i)	C II
$\mathbf{B}_{12}$	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_3 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(6i)	C II
$\mathbf{B}_{13}$	$= -x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2$	$=$	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}}$	(6i)	C II
$\mathbf{B}_{14}$	$= 2x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(6i)	C II
$\mathbf{B}_{15}$	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{3} \mathbf{a}_3$	$=$	$\sqrt{3}ax_3 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(6i)	C II
$\mathbf{B}_{16}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(12k)	C III
$\mathbf{B}_{17}$	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{3}c(3z_4 + 2) \hat{\mathbf{z}}$	(12k)	C III
$\mathbf{B}_{18}$	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{3}) \hat{\mathbf{z}}$	(12k)	C III
$\mathbf{B}_{19}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(12k)	C III
$\mathbf{B}_{20}$	$= y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{3}c(3z_4 + 2) \hat{\mathbf{z}}$	(12k)	C III
$\mathbf{B}_{21}$	$= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{3}) \hat{\mathbf{z}}$	(12k)	C III

$$\begin{aligned}
\mathbf{B}_{22} &= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - \left(z_4 - \frac{2}{3}\right) \mathbf{a}_3 &= \frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} - \frac{1}{3}c(3z_4 - 2) \hat{\mathbf{z}} &(12k) &\quad \text{C III} \\
\mathbf{B}_{23} &= (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} &(12k) &\quad \text{C III} \\
\mathbf{B}_{24} &= -x_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - \left(z_4 - \frac{1}{3}\right) \mathbf{a}_3 &= -\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{3}\right) \hat{\mathbf{z}} &(12k) &\quad \text{C III} \\
\mathbf{B}_{25} &= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - \left(z_4 - \frac{2}{3}\right) \mathbf{a}_3 &= -\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} - \frac{1}{3}c(3z_4 - 2) \hat{\mathbf{z}} &(12k) &\quad \text{C III} \\
\mathbf{B}_{26} &= -(x_4 - y_4) \mathbf{a}_1 + y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= \frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} &(12k) &\quad \text{C III} \\
\mathbf{B}_{27} &= x_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 - \left(z_4 - \frac{1}{3}\right) \mathbf{a}_3 &= \frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{3}\right) \hat{\mathbf{z}} &(12k) &\quad \text{C III}
\end{aligned}$$

References

- [1] N. Rey, P. Toulemonde, D. Machon, L. Duclaux, S. L. Floch, V. Pischedda, J. P. Itié, A.-M. Flank, P. Lagarde, W. A. Crichton, M. Mezouar, T. Strässle, D. Sheptyakov, G. Montagnac, and A. San-Miguel, *High-pressure behavior of CsC₈ graphite intercalation compound: Lattice structures and phase-transition mechanism*, Phys. Rev. B **77**, 125433 (2008), doi:10.1103/PhysRevB.77.125433.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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.