# $CsC_8$ Structure: A8B_hP27_180_2ik_d-001

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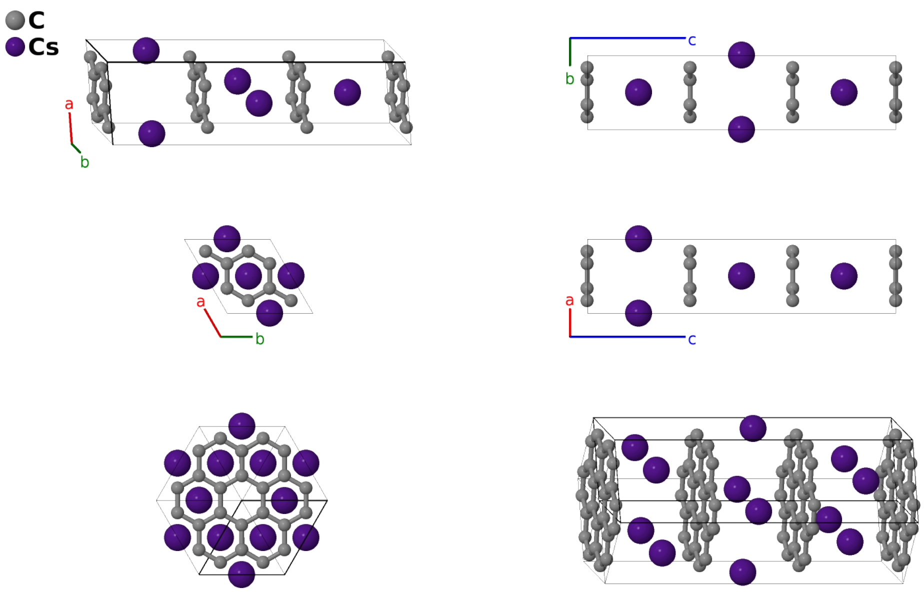
https://aflow.org/p/T338

https://aflow.org/p/A8B_hP27_180_2ik_d-001




| | |
|---|---|
| **Prototype** | $C_8Cs$ |
| **AFLOW prototype label** | A8B_hP27_180_2ik_d-001 |
| **ICSD** | none |
| **Pearson symbol** | hP27 |
| **Space group number** | 180 |
| **Space group symbol** | $P6_222$ |
| **AFLOW prototype command** | `aflow --proto=A8B_hP27_180_2ik_d-001 --params=`$a, c/a, x_2, x_3, x_4, y_4, z_4$ |

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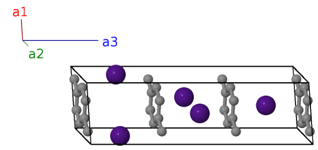
- This is the ambient pressure structure structure of $CsC_8$. Above 1.2 GPa it transforms into an orthorhombic structure which was not determined by (Rey, 2008). Further transitions occur at higher temperatures.
- This compound can also be found in the enantiomorphic space group $P6_422$ #181. To make 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

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$




## 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 |
| $\mathbf{B_{16}}$ | = | $x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\left(x_4 + y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (12k) | C III |
| $\mathbf{B_{17}}$ | = | $-y_4\,\mathbf{a}_1 + \left(x_4 - y_4\right)\,\mathbf{a}_2 + \left(z_4 + \frac{2}{3}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\left(x_4 - 2y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{3}c\left(3z_4 + 2\right)\,\hat{\mathbf{z}}$ | (12k) | C III |
| $\mathbf{B_{18}}$ | = | $-\left(x_4 - y_4\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{3}\right)\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\left(2x_4 - y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$ | (12k) | C III |
| $\mathbf{B_{19}}$ | = | $-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\left(x_4 + y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (12k) | C III |
| $\mathbf{B_{20}}$ | = | $y_4\,\mathbf{a}_1 - \left(x_4 - y_4\right)\,\mathbf{a}_2 + \left(z_4 + \frac{2}{3}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\left(-x_4 + 2y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{3}c\left(3z_4 + 2\right)\,\hat{\mathbf{z}}$ | (12k) | C III |
| $\mathbf{B_{21}}$ | = | $\left(x_4 - y_4\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{3}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\left(2x_4 - y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$ | (12k) | C III |
| $\mathbf{B_{22}}$ | = | $y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - \left(z_4 - \frac{2}{3}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\left(x_4 + y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\,\hat{\mathbf{y}} - \frac{1}{3}c\left(3z_4 - 2\right)\,\hat{\mathbf{z}}$ | (12k) | C III |
| $\mathbf{B_{23}}$ | = | $\left(x_4 - y_4\right)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\left(x_4 - 2y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$ | (12k) | C III |
| $\mathbf{B_{24}}$ | = | $-x_4\,\mathbf{a}_1 - \left(x_4 - y_4\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{3}\right)\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\left(2x_4 - y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{3}\right)\,\hat{\mathbf{z}}$ | (12k) | C III |
| $\mathbf{B_{25}}$ | = | $-y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - \left(z_4 - \frac{2}{3}\right)\,\mathbf{a}_3$ | = | $-\frac{1}{2}a\left(x_4 + y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\,\hat{\mathbf{y}} - \frac{1}{3}c\left(3z_4 - 2\right)\,\hat{\mathbf{z}}$ | (12k) | C III |
| $\mathbf{B_{26}}$ | = | $-\left(x_4 - y_4\right)\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$ | = | $\frac{1}{2}a\left(-x_4 + 2y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$ | (12k) | C III |
| $\mathbf{B_{27}}$ | = | $x_4\,\mathbf{a}_1 + \left(x_4 - y_4\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{3}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\left(2x_4 - y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{3}\right)\,\hat{\mathbf{z}}$ | (12k) | C III |

## 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* $CsC_8$ *graphite intercalation compound: Lattice structures and phase-transition mechanism*, Phys. Rev. B **77**, 125433 (2008), doi:10.1103/PhysRevB.77.125433.