

Hexagonal Graphite (A9) Structure: A_hP4_194_bc-001

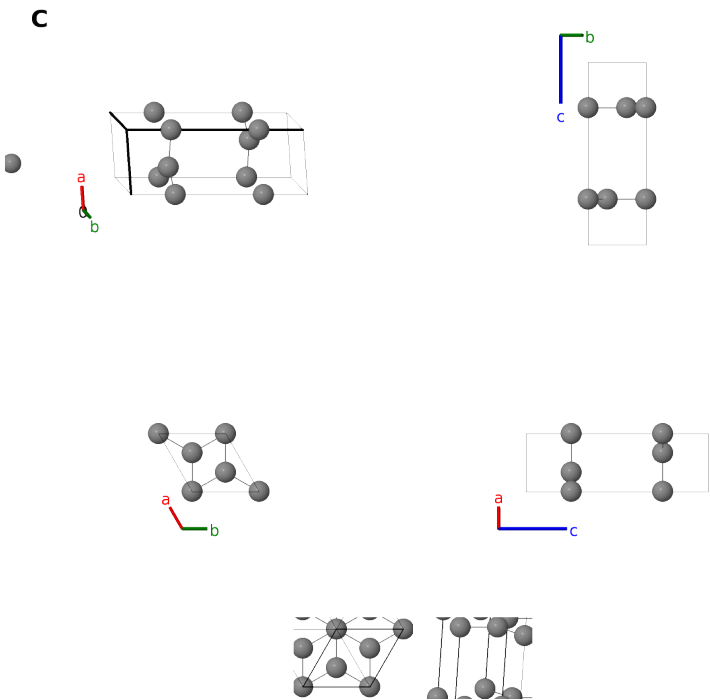
This structure previously used the label(s) **A_hP4_194_bc**. Calls to these addresses will be redirected here.

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/W4SC>

https://aflow.org/prototype-encyclopedia/A_hP4_194_bc-001



Prototype	C
AFLOW prototype label	A_hP4_194_bc-001
<i>Strukturbericht</i> designation	A9
Mineral name	graphite
ICSD	76767
CCDC	1637294
Pearson symbol	hP4
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=A_hP4_194_bc-001 --params=a, c/a</code>

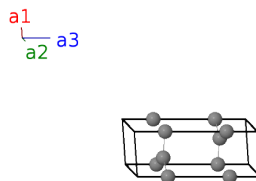
Other compounds with this structure

LiB

- According to (Wyckoff, 1963), hexagonal graphite may be either flat, space group $P6_3/mmc$ #194 (this structure) or buckled, space group $P6_3mc$ #186. We assign the *A9 Strukturbericht* designation to the unbuckled structure shown here.
 - Experimentally, a rhombohedral ($R\bar{3}m$) graphite structure is also observed.
 - Carbon can also be found in nature as cubic diamond (*A4*), lonsdaleite (hexagonal diamond, and buckminsterfullerene (C_{60}).
-

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
$\mathbf{B}_1$	$= \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}c\hat{\mathbf{z}}$	(2b)	C I
$\mathbf{B}_2$	$= \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}c\hat{\mathbf{z}}$	(2b)	C I
$\mathbf{B}_3$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(2c)	C II
$\mathbf{B}_4$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{3}{4}c\hat{\mathbf{z}}$	(2c)	C II

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017