Hexagonal Graphite ($A9$) Structure: A_hP4_194_bc-001

This structure originally had the label `A_hP4_194_bc`. Calls to that address will be redirected here.

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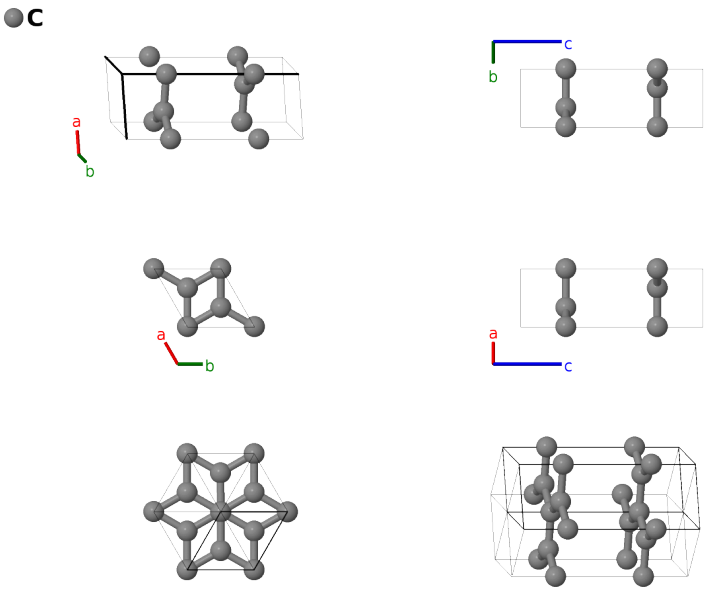
https://aflow.org/p/W4SC

https://aflow.org/p/A_hP4_194_bc-001



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

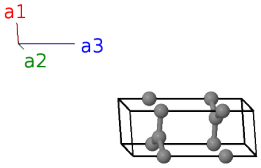
Other compounds with this structure
LiB

- According to (Wyckoff, 1963), hexagonal graphite may be either flat, space group $P6_3/mmc$ #194 or buckled, space group $P6_3mc$ #186. If it is buckled, the buckling parameter is small, less than 1/20 of the "c" parameter of the hexagonal unit cell. We assign the $A9$ *Strukturbericht* designation to the unbuckled structure shown here.

- Experimentally, a rhombohedral ($R\bar{3}m$) graphite structure is also observed.

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
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(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

References

[1] P. Trucano and R. Chen, *Structure of graphite by neutron diffraction*, Nature **258**, 136–137 (1975), doi:10.1038/258136a0.

[2] R. G. W. Wyckoff, *Crystal Structure*, vol. 1 (Interscience, New York, London, Sydney, 1963).

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).