

Buckled Graphite Structure: A_hP4_186_ab-001

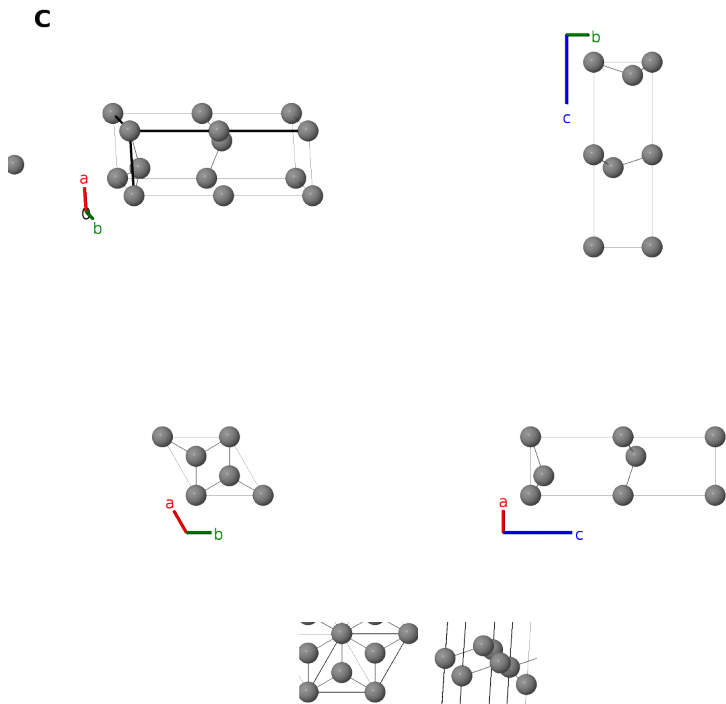
This structure previously used the label(s) **A_hP4_186_ab**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/F6SX>

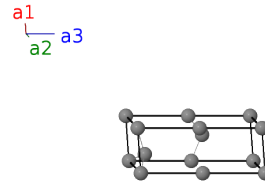
https://aflow.org/prototype-encyclopedia/A_hP4_186_ab-001



Prototype	C
AFLOW prototype label	A_hP4_186_ab-001
Mineral name	graphite
ICSD	31170
CCDC	1605322
Pearson symbol	hP4
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	<code>aflow --proto=A_hP4_186_ab-001 --params=a, c/a, z₁, z₂</code>

- According to (Wyckoff, 1963), hexagonal graphite may be either flat, space group $P6_3/mmc$ #194 or buckled, space group $P6_3mc$ #186 (this structure). “If it is buckled, the buckling parameter is small, less than 1/20 of the ‘c’ parameter of the hexagonal unit cell.” We will assign the *A9* Strukturbericht designation to the unbuckled structure.
- Experimentally, a rhombohedral ($R\bar{3}m$ #166) graphite structure is also observed.
- There is no ICSD entry for (Hull, 1917). Instead we provide the ICSD entry for the somewhat later work of (Hassel, 1924). The two structures have similar volumes and c/a values, but Hull’s value of $z_2=0.07143$ is substantially larger than Hassel and Mark’s value of 0.005. We show the former value to emphasize the buckling.
- When $z_2 = z_1$, this structure is equivalent to unbuckled (*A9*) hexagonal graphite.
- Space group $P6_3mc$ #186 is polar and does not specify the origin of the z -axis. Here we chose $z_1 = 0$ for the carbon (2a) site.

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
$\mathbf{B}_1$	$z_1 \mathbf{a}_3$	=	$cz_1 \hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B}_2$	$(z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B}_3$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2b)	C II
$\mathbf{B}_4$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	C II

References

- [1] A. W. Hull, *A New Method of X-Ray Crystal Analysis*, Phys. Rev. **10**, 661–696 (1917), doi:10.1103/PhysRev.10.661.
- [2] O. Hassel and H. Mark, *Über die Kristallstruktur des Graphits*, Z. f. Physik **25**, 317–337 (1924), doi:10.1007/BF01327534.

Found in

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

First cited in

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