Buckled Graphite Structure: A_hP4_186_ab-001

This structure originally had the label `A_hP4_186_ab`. Calls to that address will be redirected here.

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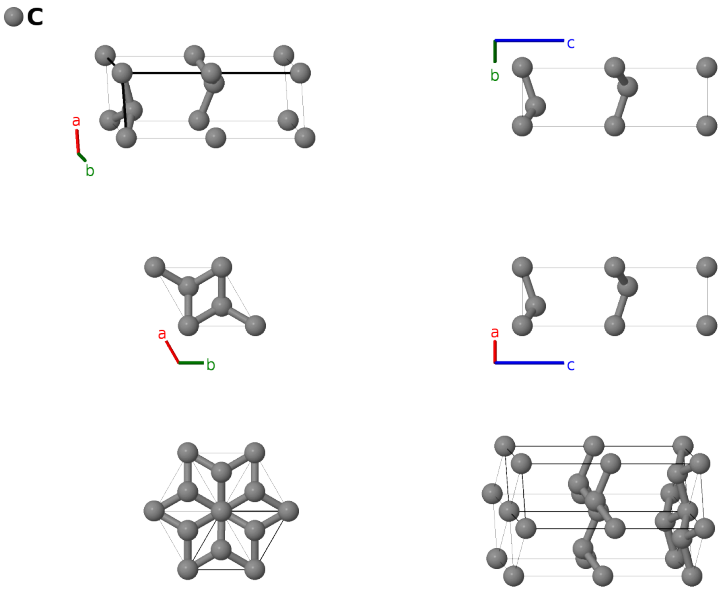
https://aflow.org/p/F6SX

https://aflow.org/p/A_hP4_186_ab-001



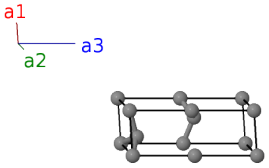
Prototype	C
AFLOW prototype label	A_hP4_186_ab-001
Mineral name	graphite
ICSD	31170
Pearson symbol	hP4
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	`aflow --proto=A_hP4_186_ab-001 --params=`$a, c/a, z_1, z_2$

- 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 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 does not specify the origin of the z-axis. Here we chose $z_1 = 0$ for the carbon (2a) site.

Hexagonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B_2}$	=	$\left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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).