Rhombohedral Graphite Structure: A_hR2_166_c-002

This structure originally had the label `A_hR2_166_c.C`. Calls to that address will be redirected here.

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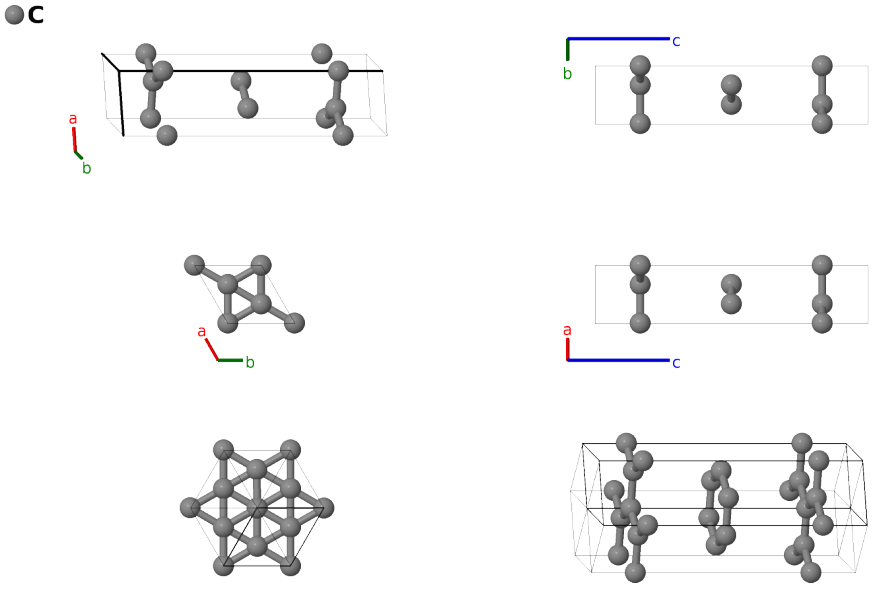
https://aflow.org/p/NXUA

https://aflow.org/p/A_hR2_166_c-002



Prototype	C
AFLOW prototype label	A_hR2_166_c-002
ICSD	31829
Pearson symbol	hR2
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A_hR2_166_c-002 --params=`$a, c/a, x_1$

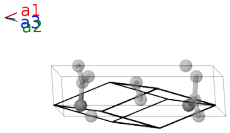
Other compounds with this structure
Bi, P, Sb

- Graphite also comes in a hexagonal form, which may be either flat (A9) or buckled. When $x_1 = 1/6$ the graphite sheets are flat, however this does not produce a change in symmetry as it does in the hexagonal graphite structures.
- All of the elements listed in the "Other compounds" list have experimental entries in the ICSD.

- α-As ($A7$), rhombohedral graphite (A_hR2_166_c), and β-O have the same AFLOW prototype label, A_hR2_166_c. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files. Hexagonal settings of rhombohedral structures can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(2c)	C I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-cx_1\,\hat{\mathbf{z}}$	(2c)	C I

References

[1] H. Lipson and A. R. Stokes, *The structure of graphite*, Proc. Roy. Soc. A **181**, 101–105 (1942), doi:10.1098/rspa.1942.0063.

Found in

[1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).