Lonsdaleite (Hexagonal Diamond) Structure: A_hP4_194_f-001

This structure originally had the label `A_hP4_194_f`. Calls to that address will be redirected here.

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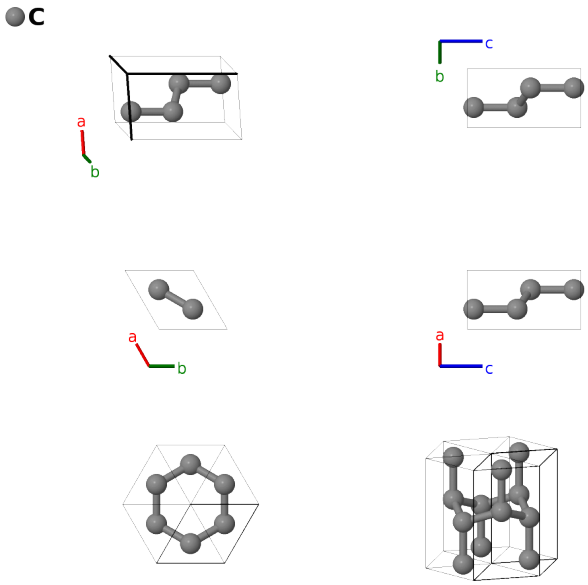
https://aflow.org/p/4AMD

https://aflow.org/p/A_hP4_194_f-001



Prototype	C
AFLOW prototype label	A_hP4_194_f-001
Mineral name	lonsdaleite
ICSD	66465
Pearson symbol	hP4
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=A_hP4_194_f-001 --params=`$a, c/a, z_1$

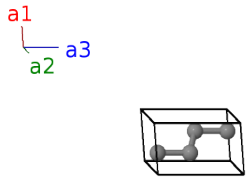
Other compounds with this structure
Ge (hexagonal), H (hexagonal), N (hexagonal), O (hexagonal), Si (hexagonal)

- Hexagonal diamond was named lonsdaleite in honor of Kathleen Lonsdale.
- This structure is related to the hcp ($A3$) structure in the same way that diamond ($A4$) is related to the fcc lattice ($A1$).
- It can also be obtained from wurtzite ($B4$) by replacing both the Zn and S atoms by carbon.

- The "ideal" structure, where the nearest-neighbor environment of each atom is the same as in diamond, is achieved when we take $c/a = \sqrt{8/3}$ and $z_1 = 1/16$.
- Alternatively, we can take $z_1 = 3/16$, in which case the origin is at the center of a C-C bond aligned in the [0001] direction.
- When $z_1 = 0$ this structure becomes a set of graphitic sheets, but not true hexagonal graphite ($A9$), as the stacking differs.
- (Yoshiasa, 2003) does not have an ICSD entry for Lonsdaleite, so we use the one provided for (Ownby, 1992).

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
$\mathbf{B_1}$	=	$\tfrac{1}{3}\,\mathbf{a}_1 + \tfrac{2}{3}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4f)	C I
$\mathbf{B_2}$	=	$\tfrac{2}{3}\,\mathbf{a}_1 + \tfrac{1}{3}\,\mathbf{a}_2 + \left(z_1 + \tfrac{1}{2}\right)\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_1 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	C I
$\mathbf{B_3}$	=	$\tfrac{2}{3}\,\mathbf{a}_1 + \tfrac{1}{3}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4f)	C I
$\mathbf{B_4}$	=	$\tfrac{1}{3}\,\mathbf{a}_1 + \tfrac{2}{3}\,\mathbf{a}_2 - \left(z_1 - \tfrac{1}{2}\right)\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_1 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	C I

References

[1] A. Yoshiasa, Y. Murai, O. Ohtaka, and T. Katsura, *Detailed Structures of Hexagonal Diamond (lonsdaleite) and Wurtzite-type BN*, Jpn. J. Appl. Phys. **42**, 1694–1704 (2003), doi:10.1143/JJAP.42.1694.

[2] P. D. Ownby, X. Yang, and J. Liu, *Calculated X-ray Diffraction Data for Diamond Polytypes*, J. Am. Ceram. Soc. **75**, 1876–1883 (1992), doi:10.1111/j.1151-2916.1992.tb07211.x.