

Diamond (A4) Structure:

A_cF8_227_a-001

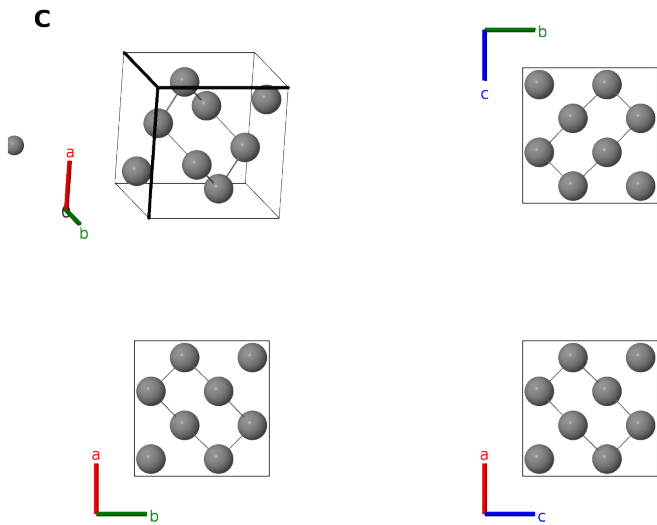
This structure previously used the label(s) **A_cF8_227_a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/X5M8>

https://aflow.org/prototype-encyclopedia/A_cF8_227_a-001



Prototype	C
AFLOW prototype label	A_cF8_227_a-001
<i>Strukturbericht</i> designation	A4
Mineral name	diamond
ICSD	53779
CCDC	1618419
Pearson symbol	cF8
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A_cF8_227_a-001 --params=a</code>

Other compounds with this structure
Ge, Si, Sn

- This is the first crystal structure to be determined by X-ray diffraction.
- Carbon can also be found in nature as graphite (A9), lonsdaleite (hexagonal diamond), and buckminsterfullerene (C₆₀).

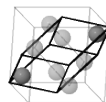
Face-centered Cubic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}$$

$\mathbf{a}_2$
 $\mathbf{a}_1$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	$\frac{1}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3$	$=$	$\frac{1}{8}a \hat{\mathbf{x}} + \frac{1}{8}a \hat{\mathbf{y}} + \frac{1}{8}a \hat{\mathbf{z}}$	(8a) C I
$\mathbf{B}_2$	$=$	$\frac{7}{8} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3$	$=$	$\frac{7}{8}a \hat{\mathbf{x}} + \frac{7}{8}a \hat{\mathbf{y}} + \frac{7}{8}a \hat{\mathbf{z}}$	(8a) C I

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