Diamond ($A4$) Structure: A_cF8_227_a-001

This structure originally had the label `A_cF8_227_a`. Calls to that address will be redirected here.

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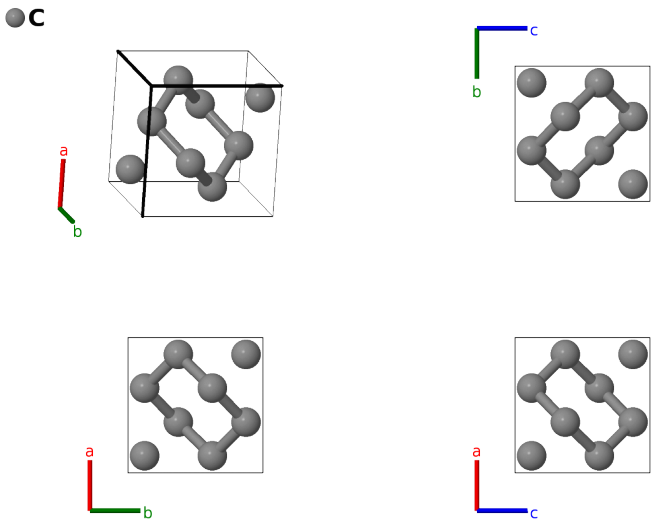
https://aflow.org/p/X5M8

https://aflow.org/p/A_cF8_227_a-001



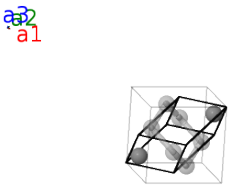
Prototype	C
AFLOW prototype label	A_cF8_227_a-001
***Strukturbericht* designation**	$A4$
Mineral name	diamond
ICSD	53779
Pearson symbol	cF8
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	`aflow --proto=A_cF8_227_a-001 --params=`a

Other compounds with this structure
Ge, Si, Sn

- This is the first crystal structure to be determined by X-ray diffraction.

Face-centered Cubic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$$



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

References

[1] W. H. Bragg and W. L. Bragg, *The Structure of Diamond*, Proc. Phys. Soc. London A **89**, 277–291 (1913), doi:10.1098/rspa.1913.0084.