

Pu₂C₃ (*D*5_{*c*}) Structure: A3B2_cI40_220_d_c-001

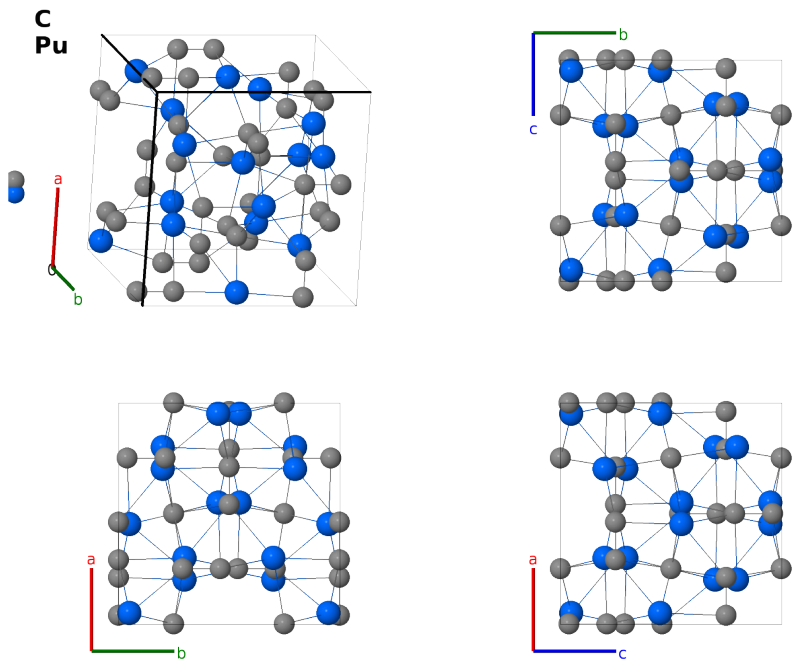
This structure previously used the label(s) A3B2_cI40_220_d.c. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/M1ZX>

https://aflow.org/prototype-encyclopedia/A3B2_cI40_220_d_c-001



Prototype	C ₃ Pu ₂
AFLOW prototype label	A3B2_cI40_220_d_c-001
<i>Strukturbericht</i> designation	<i>D</i> 5 _{<i>c</i>}
ICSD	16511
CCDC	1597085
Pearson symbol	cI40
Space group number	220
Space group symbol	<i>I</i> $\bar{4}$ 3 <i>d</i>
AFLOW prototype command	<code>aflow --proto=A3B2_cI40_220_d_c-001</code> <code>--params=<i>a</i>, <i>x</i>₁, <i>x</i>₂</code>

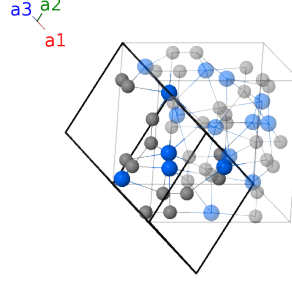
Other compounds with this structure

Am_2C_3 , Ce_2C_3 , Dy_2C_3 , Ho_2C_3 , Hf_2C_3 , La_2C_3 , Nd_2C_3 , Np_2C_3 , Pr_2C_3 , Pu_2C_3 , Sm_2C_3 , Th_2C_3 , U_2C_3 , Y_2C_3 , Cs_2O_3 , Ru_2Er_3 , Rb_2O_3 , Ru_2Y_3

- We use the data for ^{240}Pu .

Body-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - \frac{1}{2}a\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 2x_1 \mathbf{a}_1 + 2x_1 \mathbf{a}_2 + 2x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(16c)	Pu I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 - (2x_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(16c)	Pu I
$\mathbf{B}_3$	$= -(2x_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(16c)	Pu I
$\mathbf{B}_4$	$= -(2x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(16c)	Pu I
$\mathbf{B}_5$	$= (2x_1 + \frac{1}{2}) \mathbf{a}_1 + (2x_1 + \frac{1}{2}) \mathbf{a}_2 + (2x_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{y}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(16c)	Pu I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 - 2x_1 \mathbf{a}_3$	$=$	$-a(x_1 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_1 - \frac{1}{4}) \hat{\mathbf{y}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(16c)	Pu I
$\mathbf{B}_7$	$= -2x_1 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$a(x_1 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_1 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_1 - \frac{1}{4}) \hat{\mathbf{z}}$	(16c)	Pu I
$\mathbf{B}_8$	$= -2x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(16c)	Pu I
$\mathbf{B}_9$	$= \frac{1}{4} \mathbf{a}_1 + (x_2 + \frac{1}{4}) \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{10}$	$= \frac{3}{4} \mathbf{a}_1 - (x_2 - \frac{1}{4}) \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{11}$	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (x_2 + \frac{1}{4}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(24d)	C I
$\mathbf{B}_{12}$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (x_2 - \frac{1}{4}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{13}$	$= (x_2 + \frac{1}{4}) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{14}$	$= -(x_2 - \frac{1}{4}) \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{15}$	$= (x_2 + \frac{3}{4}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + a(x_2 + \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{16}$	$= -(x_2 - \frac{3}{4}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-\frac{1}{4}a \hat{\mathbf{x}} - a(x_2 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{17}$	$= \frac{3}{4} \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + (x_2 + \frac{3}{4}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{18}$	$= \frac{1}{4} \mathbf{a}_1 - x_2 \mathbf{a}_2 - (x_2 - \frac{3}{4}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{4}a \hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B}_{19}$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{3}{4}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + a(x_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(24d)	C I

$$\mathbf{B}_{20} = -x_2 \mathbf{a}_1 - \left(x_2 - \frac{3}{4}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 = \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{4}a \hat{\mathbf{y}} - a \left(x_2 - \frac{1}{4}\right) \hat{\mathbf{z}} \quad (24d) \quad \text{C I}$$

References

- [1] J. L. Green, G. P. Arnold, J. A. Leary, and N. G. Nereson, *Crystallographic and magnetic ordering studies of plutonium carbides using neutron diffraction*, J. Nucl. Mater. **34**, 281–289 (1970), doi:10.1016/0022-3115(70)90194-7.

Found in

- [1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.

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