Pu_2C_3 ($D5_c$) Structure: A3B2_cI40_220_d_c-001

This structure originally had the label `A3B2_cI40_220_d_c`. Calls to that address will be redirected here.

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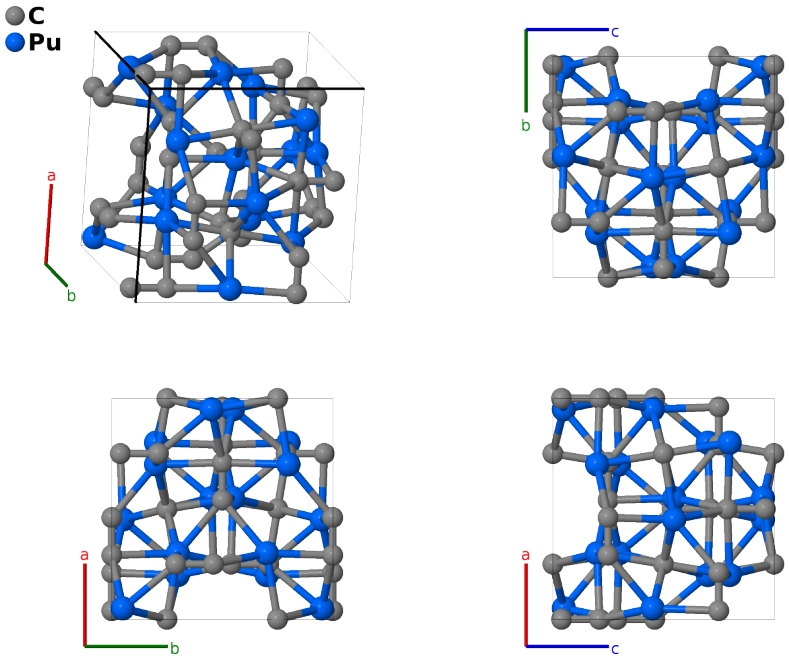
https://aflow.org/p/M1ZX

https://aflow.org/p/A3B2_cI40_220_d_c-001



Prototype	C_3Pu_2
AFLOW prototype label	A3B2_cI40_220_d_c-001
***Strukturbericht* designation**	$D5_c$
ICSD	16511
Pearson symbol	cI40
Space group number	220
Space group symbol	$I\bar{4}3d$
AFLOW prototype command	`aflow --proto=A3B2_cI40_220_d_c-001 --params=`a, x_1, x_2

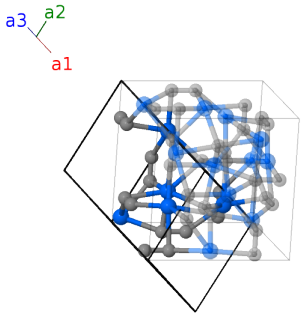
Other compounds with this structure

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

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



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
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(2x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(16c)	Pu I
$\mathbf{B_3}$	=	$-\left(2x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(16c)	Pu I
$\mathbf{B_4}$	=	$-\left(2x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16c)	Pu I
$\mathbf{B_5}$	=	$\left(2x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(2x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(2x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	Pu I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - 2x_1\,\mathbf{a}_3$	=	$-a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	Pu I
$\mathbf{B_7}$	=	$-2x_1\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	Pu I
$\mathbf{B_8}$	=	$-2x_1\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16c)	Pu I
$\mathbf{B_9}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B_{10}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B_{11}}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(24d)	C I
$\mathbf{B_{12}}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B_{13}}$	=	$\left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B_{14}}$	=	$-\left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B_{15}}$	=	$\left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B_{16}}$	=	$-\left(x_2 - \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B_{17}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B_{18}}$	=	$\frac{1}{4}\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - \left(x_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - \frac{1}{4}a\,\hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B_{19}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(24d)	C I
$\mathbf{B_{20}}$	=	$-x_2\,\mathbf{a}_1 - \left(x_2 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(24d)	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.

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