Dy_5Pd_2 Structure: A7B2_cF144_227_2ef_e-001

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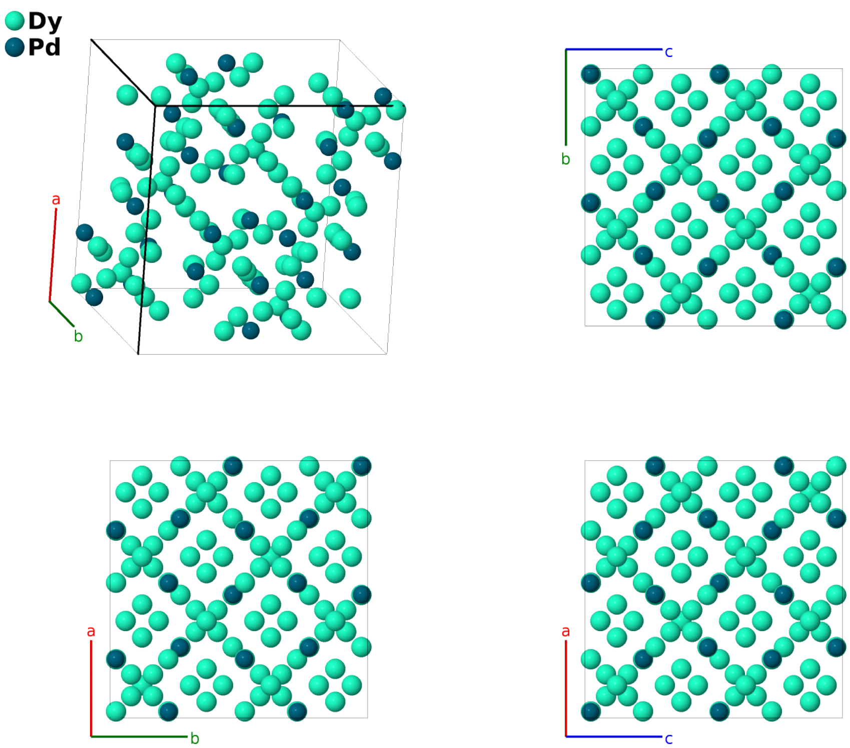
https://aflow.org/p/WYVV

https://aflow.org/p/A7B2_cF144_227_2ef_e-001



Prototype	Dy_5Pd_2
AFLOW prototype label	A7B2_cF144_227_2ef_e-001
ICSD	103347
Pearson symbol	cF144
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	`aflow --proto=A7B2_cF144_227_2ef_e-001` `--params=`a, x_1, x_2, x_3, x_4

Other compounds with this structure
Er_5Pd_2, Ho_5Pd_2, Lu_5Pd_2, Tb_5Pd_2, Tm_5Pd_2, Y_5Pd_2

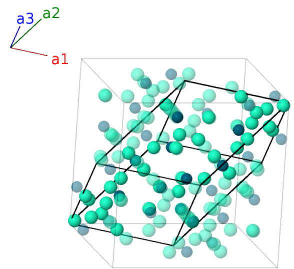
- There is considerable disorder in this structure, with all of the (32e) sites having vacancies:
  - The Dy-I site is 50% occupied.

- The Dy-II site is 12.5% occupied
- The Pd site is 87.5% occupied.

- This gives a composition of $Dy_{2.43}Pd$.

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(32e)	Dy I
$\mathbf{B_2}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 - \left(3x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(32e)	Dy I
$\mathbf{B_3}$	=	$x_1\,\mathbf{a}_1 - \left(3x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Dy I
$\mathbf{B_4}$	=	$-\left(3x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Dy I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(3x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(32e)	Dy I
$\mathbf{B_6}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(32e)	Dy I
$\mathbf{B_7}$	=	$-x_1\,\mathbf{a}_1 + \left(3x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Dy I
$\mathbf{B_8}$	=	$\left(3x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Dy I
$\mathbf{B_9}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(32e)	Dy II
$\mathbf{B_{10}}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - \left(3x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(32e)	Dy II
$\mathbf{B_{11}}$	=	$x_2\,\mathbf{a}_1 - \left(3x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Dy II
$\mathbf{B_{12}}$	=	$-\left(3x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Dy II
$\mathbf{B_{13}}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(3x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(32e)	Dy II
$\mathbf{B_{14}}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(32e)	Dy II
$\mathbf{B_{15}}$	=	$-x_2\,\mathbf{a}_1 + \left(3x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Dy II
$\mathbf{B_{16}}$	=	$\left(3x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Dy II
$\mathbf{B_{17}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(32e)	Pd I
$\mathbf{B_{18}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(3x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(32e)	Pd I
$\mathbf{B_{19}}$	=	$x_3\,\mathbf{a}_1 - \left(3x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Pd I
$\mathbf{B_{20}}$	=	$-\left(3x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Pd I
$\mathbf{B_{21}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(3x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(32e)	Pd I
$\mathbf{B_{22}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(32e)	Pd I
$\mathbf{B_{23}}$	=	$-x_3\,\mathbf{a}_1 + \left(3x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Pd I
$\mathbf{B_{24}}$	=	$\left(3x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32e)	Pd I
$\mathbf{B_{25}}$	=	$-\left(x_4 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Dy III

$\mathbf{B_{26}}$	=	$x_4\,\mathbf{a}_1-\left(x_4-\frac{1}{4}\right)\,\mathbf{a}_2-\left(x_4-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{8}a\,\hat{\mathbf{y}}+\frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Dy III
$\mathbf{B_{27}}$	=	$x_4\,\mathbf{a}_1-\left(x_4-\frac{1}{4}\right)\,\mathbf{a}_2+x_4\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}}+ax_4\,\hat{\mathbf{y}}+\frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Dy III
$\mathbf{B_{28}}$	=	$-\left(x_4-\frac{1}{4}\right)\,\mathbf{a}_1+x_4\,\mathbf{a}_2-\left(x_4-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}}-a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{y}}+\frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	Dy III
$\mathbf{B_{29}}$	=	$x_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2-\left(x_4-\frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}}+\frac{1}{8}a\,\hat{\mathbf{y}}+ax_4\,\hat{\mathbf{z}}$	(48f)	Dy III
$\mathbf{B_{30}}$	=	$-\left(x_4-\frac{1}{4}\right)\,\mathbf{a}_1-\left(x_4-\frac{1}{4}\right)\,\mathbf{a}_2+x_4\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}}+\frac{1}{8}a\,\hat{\mathbf{y}}-a\left(x_4-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48f)	Dy III
$\mathbf{B_{31}}$	=	$\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_1-x_4\,\mathbf{a}_2+\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}}+a\left(x_4+\frac{3}{4}\right)\,\hat{\mathbf{y}}+\frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	Dy III
$\mathbf{B_{32}}$	=	$-x_4\,\mathbf{a}_1+\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_2-x_4\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}+\frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	Dy III
$\mathbf{B_{33}}$	=	$-x_4\,\mathbf{a}_1+\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_2+\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{3}{4}\right)\,\hat{\mathbf{x}}+\frac{3}{8}a\,\hat{\mathbf{y}}+\frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	Dy III
$\mathbf{B_{34}}$	=	$\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_1-x_4\,\mathbf{a}_2-x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}+\frac{3}{8}a\,\hat{\mathbf{y}}+\frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	Dy III
$\mathbf{B_{35}}$	=	$-x_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2+\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}}+\frac{3}{8}a\,\hat{\mathbf{y}}-ax_4\,\hat{\mathbf{z}}$	(48f)	Dy III
$\mathbf{B_{36}}$	=	$\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_1+\left(x_4+\frac{3}{4}\right)\,\mathbf{a}_2-x_4\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}}+\frac{3}{8}a\,\hat{\mathbf{y}}+a\left(x_4+\frac{3}{4}\right)\,\hat{\mathbf{z}}$	(48f)	Dy III

References

[1] M. L. Fornasini and Palenzona, *Crystal structure of the so-called R.E.$_5$Pd$_2$ compounds*, J. Less-Common Met. **38**, 77–82 (1974), doi:10.1016/0022-5088(74)90205-7.