β-Hg_4Pt Structure: A4B_cI10_229_c_a-001

This structure originally had the label `A4B_cI10_229_c_a`. Calls to that address will be redirected here.

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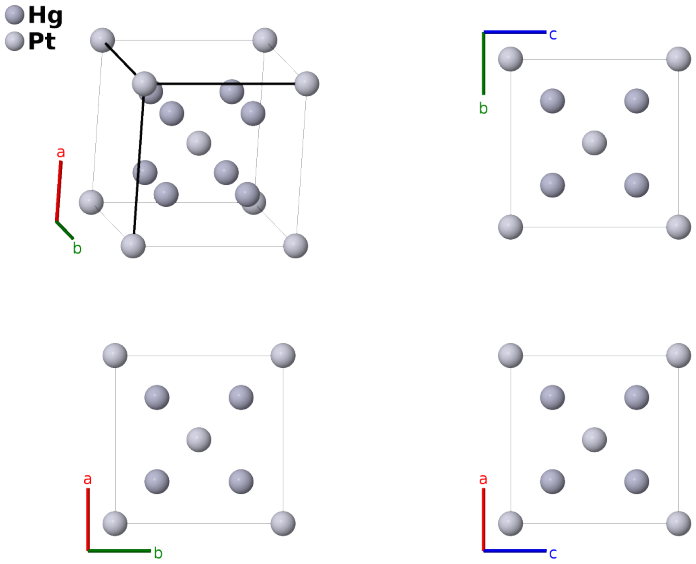
https://aflow.org/p/78LF

https://aflow.org/p/A4B_cI10_229_c_a-001



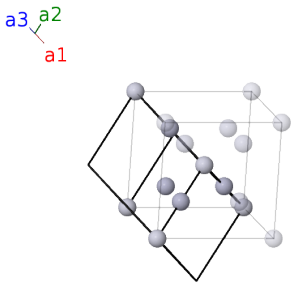
Prototype	Hg_4Pt
AFLOW prototype label	A4B_cI10_229_c_a-001
ICSD	150772
Pearson symbol	cI10
Space group number	229
Space group symbol	$Im\bar{3}m$
AFLOW prototype command	`aflow --proto=A4B_cI10_229_c_a-001 --params=`a

Other compounds with this structure
Hg_4Ni, Hg_4Pd, Hg_4U

- (Bauer, 1953) give the lattice constant in kX units. We convert this to Ångströms by multiplying that number by 1.00202 (Wood, 1947).

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Pt I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Hg I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Hg I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Hg I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Hg I

References

[1] E. Bauer, H. Nowotny, and A. Stempfl, *Röntgenographische Untersuchungen im System: Platin-Quecksilber*, Monatsh. Chem. **84**, 211–212 (1953), doi:10.1007/BF00899140.

[2] E. A. Wood, *The Conversion Factor for kX Units to Angström Units*, J. App. Phys. **18**, 929–930 (1947), doi:10.1063/1.1697570.

Found in

[1] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, *International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 4 (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfort, 1958), 1964 reprint with corrections edn.