TaRh Structure: AB_oP12_51_ei_fj-001

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https://aflow.org/p/1M54

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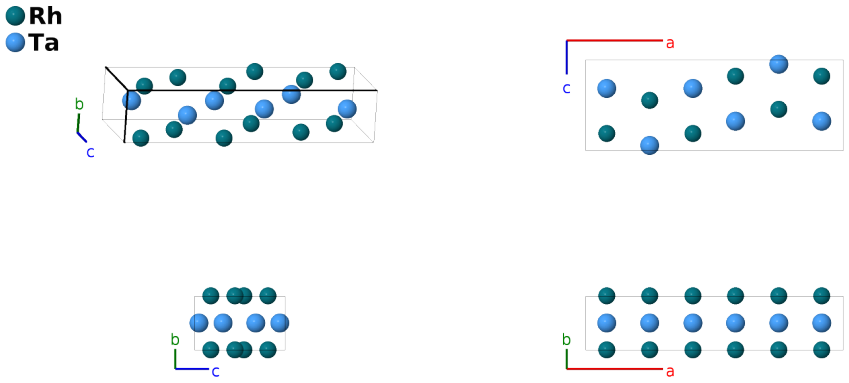


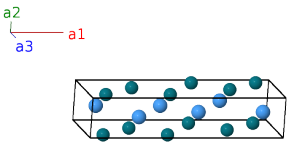
Prototype	RhTa
AFLOW prototype label	AB_oP12_51_ei_fj-001
ICSD	105938
Pearson symbol	oP12
Space group number	51
Space group symbol	*Pmma*
AFLOW prototype command	`aflow --proto=AB_oP12_51_ei_fj-001 --params=`$a, b/a, c/a, z_1, z_2, x_3, z_3, x_4, z_4$

Other compounds with this structure
NbIr, TaIr, NbRh

- (Giessen, 1964) give the actual composition as $(Ta_{0.79}Rh_{0.21})Rh$, with similar compositions for the related compounds.
- (Pearson, 1967) and others refer to this as α_1-TaRh.
- (Giessen, 1964) give the structure in the *Pmcm* setting of space group #51. We used FINDSYM to transform this to the standard *Pmma* setting.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + z_1\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + cz_1\,\hat{\mathbf{z}}$	(2e)	Rh I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 - z_1\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - cz_1\,\hat{\mathbf{z}}$	(2e)	Rh I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2f)	Ta I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2f)	Ta I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(4i)	Rh II
$\mathbf{B_6}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(4i)	Rh II
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - cz_3\,\hat{\mathbf{z}}$	(4i)	Rh II
$\mathbf{B_8}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - cz_3\,\hat{\mathbf{z}}$	(4i)	Rh II
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4j)	Ta II
$\mathbf{B_{10}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4j)	Ta II
$\mathbf{B_{11}}$	=	$-x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4j)	Ta II
$\mathbf{B_{12}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4j)	Ta II

References

[1] B. C. Giessen and N. J. Grant, *New intermediate phases in system of Nb or Ta with Rh, Ir, Pd, or Pt*, Acta Cryst. **17**, 615–616 (1964), doi:10.1107/S0365110X64001438.

Found in

[1] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, Volume 2*, *International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 8 (Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1967).