

TaRh Structure:

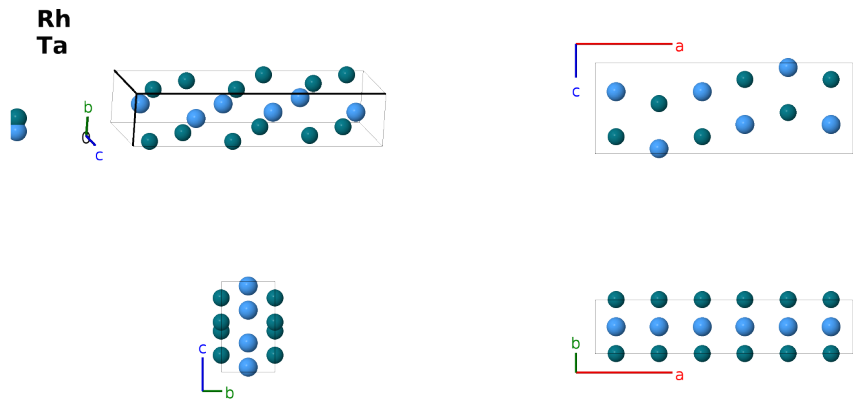
AB_oP12_51_ei_fj-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/1M54>

https://aflow.org/prototype-encyclopedia/AB_oP12_51_ei_fj-001



Prototype	RhTa
AFLOW prototype label	AB_oP12_51_ei_fj-001
ICSD	105938
CCDC	1663804
Pearson symbol	oP12
Space group number	51
Space group symbol	$Pmma$
AFLOW prototype command	<code>aflow --proto=AB_oP12_51_ei_fj-001</code> <code>--params=$a, b/a, c/a, z_1, z_2, x_3, z_3, x_4, z_4$</code>

Other compounds with this structure

NbIr, TaIr, NbRh

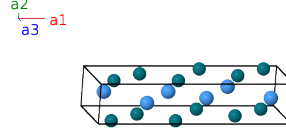
- (Giessen, 1964) give the actual composition as $(\text{Ta}_{0.79}\text{Rh}_{0.21})\text{Rh}$, with similar compositions for the related compounds.
- (Pearson, 1967) and others refer to this as $\alpha_1\text{-TaRh}$.
- (Giessen, 1964) give the structure in the $Pmcm$ setting of space group #51. We 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).

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