$Hf_{10}Ta_3S_3$ Structure: A11B3C2_cI64_197_cdf_e_c-001

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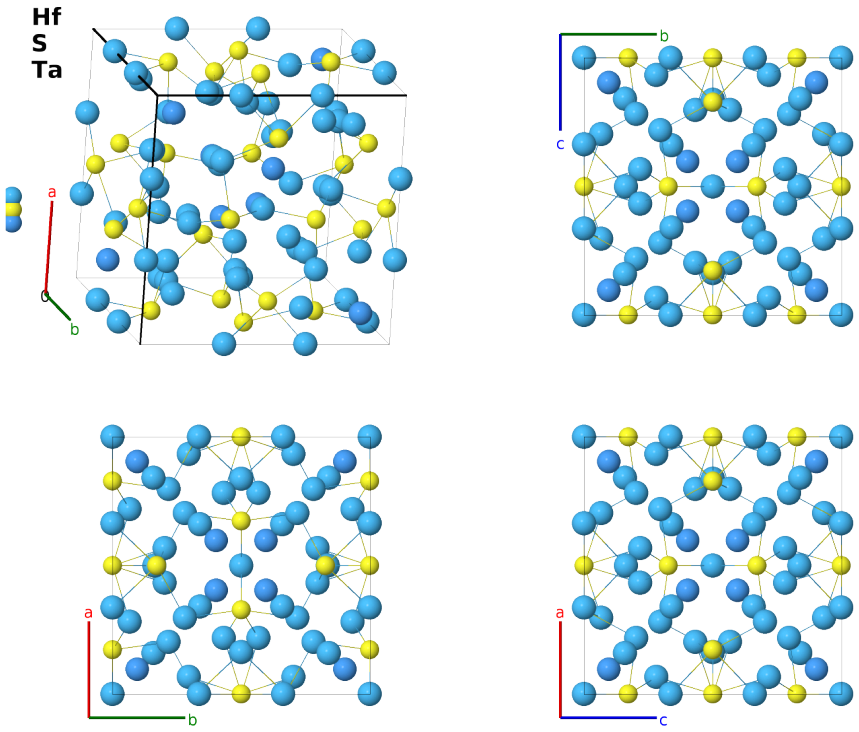
https://aflow.org/prototype-encyclopedia/8883

https://aflow.org/prototype-encyclopedia/A11B3C2_cI64_197_cdf_e_c-001



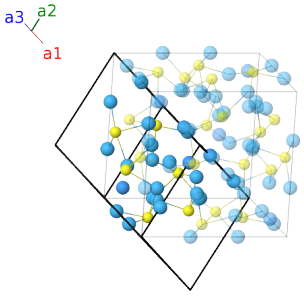
Prototype	$Hf_{10}S_3Ta_3$
AFLOW prototype label	A11B3C2_cI64_197_cdf_e_c-001
ICSD	73743
CCDC	1634504
Pearson symbol	cI64
Space group number	197
Space group symbol	$I23$
AFLOW prototype command	`aflow --proto=A11B3C2_cI64_197_cdf_e_c-001 --params=`$a, x_1, x_2, x_3, x_4, x_5, y_5, z_5$

Other compounds with this structure
$Hf_9ZrTa_3S_3$, $Hf_{10}TeNb_2S_3$

- The metallic sites are mixed. While both (Marking, 1993) and (Villars, 2016) assign the Hf II, Hf III and Ta sites as we have, (Marking, 1993) assumes that what we call the Hf I site (their M2 site) is approximately 55% hafnium and 45% tantalum, making the nominal composition $Hf_{10.1}Ta_{2.9}S_3$.

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
$\mathbf{B_1}$	=	$2x_1\,\mathbf{a}_1 + 2x_1\,\mathbf{a}_2 + 2x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(8c)	Hf I
$\mathbf{B_2}$	=	$-2x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(8c)	Hf I
$\mathbf{B_3}$	=	$-2x_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(8c)	Hf I
$\mathbf{B_4}$	=	$-2x_1\,\mathbf{a}_1$	=	$ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(8c)	Hf I
$\mathbf{B_5}$	=	$2x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + 2x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	Ta I
$\mathbf{B_6}$	=	$-2x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	Ta I
$\mathbf{B_7}$	=	$-2x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	Ta I
$\mathbf{B_8}$	=	$-2x_2\,\mathbf{a}_1$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	Ta I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(12d)	Hf II
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(12d)	Hf II
$\mathbf{B_{11}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{y}}$	(12d)	Hf II
$\mathbf{B_{12}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{y}}$	(12d)	Hf II
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{z}}$	(12d)	Hf II
$\mathbf{B_{14}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{z}}$	(12d)	Hf II
$\mathbf{B_{15}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(12e)	S I
$\mathbf{B_{16}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(12e)	S I
$\mathbf{B_{17}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12e)	S I
$\mathbf{B_{18}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12e)	S I
$\mathbf{B_{19}}$	=	$x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{z}}$	(12e)	S I
$\mathbf{B_{20}}$	=	$-x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{z}}$	(12e)	S I
$\mathbf{B_{21}}$	=	$(y_5 + z_5)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + (x_5 + y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}}$	(24f)	Hf III
$\mathbf{B_{22}}$	=	$-(y_5 - z_5)\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - (x_5 + y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}}$	(24f)	Hf III
$\mathbf{B_{23}}$	=	$(y_5 - z_5)\,\mathbf{a}_1 - (x_5 + z_5)\,\mathbf{a}_2 - (x_5 - y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}}$	(24f)	Hf III

$$\mathbf{B_{24}} = -(y_5+z_5)\,\mathbf{a}_1+(x_5-z_5)\,\mathbf{a}_2+(x_5-y_5)\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}-az_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{Hf III}$$

$$\mathbf{B_{25}} = (x_5+y_5)\,\mathbf{a}_1+(y_5+z_5)\,\mathbf{a}_2+(x_5+z_5)\,\mathbf{a}_3 = az_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}+ay_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{Hf III}$$

$$\mathbf{B_{26}} = -(x_5+y_5)\,\mathbf{a}_1-(y_5-z_5)\,\mathbf{a}_2-(x_5-z_5)\,\mathbf{a}_3 = az_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}-ay_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{Hf III}$$

$$\mathbf{B_{27}} = -(x_5-y_5)\,\mathbf{a}_1+(y_5-z_5)\,\mathbf{a}_2-(x_5+z_5)\,\mathbf{a}_3 = -az_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+ay_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{Hf III}$$

$$\mathbf{B_{28}} = (x_5-y_5)\,\mathbf{a}_1-(y_5+z_5)\,\mathbf{a}_2+(x_5-z_5)\,\mathbf{a}_3 = -az_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}-ay_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{Hf III}$$

$$\mathbf{B_{29}} = (x_5+z_5)\,\mathbf{a}_1+(x_5+y_5)\,\mathbf{a}_2+(y_5+z_5)\,\mathbf{a}_3 = ay_5\,\hat{\mathbf{x}}+az_5\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{Hf III}$$

$$\mathbf{B_{30}} = -(x_5-z_5)\,\mathbf{a}_1-(x_5+y_5)\,\mathbf{a}_2-(y_5-z_5)\,\mathbf{a}_3 = -ay_5\,\hat{\mathbf{x}}+az_5\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{Hf III}$$

$$\mathbf{B_{31}} = -(x_5+z_5)\,\mathbf{a}_1-(x_5-y_5)\,\mathbf{a}_2+(y_5-z_5)\,\mathbf{a}_3 = ay_5\,\hat{\mathbf{x}}-az_5\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{Hf III}$$

$$\mathbf{B_{32}} = (x_5-z_5)\,\mathbf{a}_1+(x_5-y_5)\,\mathbf{a}_2-(y_5+z_5)\,\mathbf{a}_3 = -ay_5\,\hat{\mathbf{x}}-az_5\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}} \quad (24f) \quad \text{Hf III}$$

References

[1] G. A. Marking and H. F. Franzen, *Hafnium tantalum sulfide ($Hf_{10}Ta_3S_3$), a new structure type related to γ-brass: confirmation of Hume-Rothery and Brewer-Engel electron concentration rules*, J. Am. Chem. Soc. **115**, 6126–6130 (1993), doi:10.1021/ja00067a030.

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First cited in

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