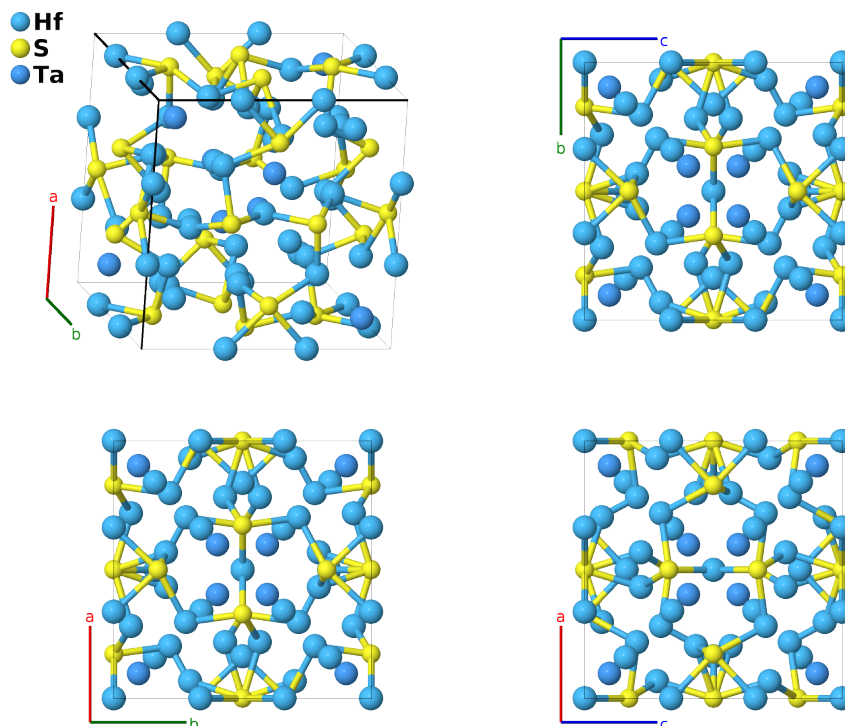


Hf₁₀Ta₃S₃ Structure: A11B3C2_cI64_197_cdf_e_c-001

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<https://aflow.org/p/8883>

https://aflow.org/p/A11B3C2_cI64_197_cdf_e_c-001



Prototype	Hf ₁₀ S ₃ Ta ₃
AFLOW prototype label	A11B3C2_cI64_197_cdf_e_c-001
ICSD	73743
Pearson symbol	cI64
Space group number	197
Space group symbol	<i>I</i> 23
AFLOW prototype command	<code>aflow --proto=A11B3C2_cI64_197_cdf_e_c-001 --params=a, x₁, x₂, x₃, x₄, x₅, y₅, z₅</code>

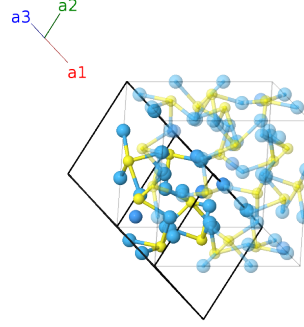
Other compounds with this structure

Hf₉ZrTa₃S₃, Hf₁₀TeNb₂S₃

- 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}S₃.

Body-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{2}a \hat{\mathbf{z}}\end{aligned}$$



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}	$= \frac{1}{2} \mathbf{a}_1 + x_4 \mathbf{a}_2 + (x_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}$	(12e)	S I
\mathbf{B}_{16}	$= \frac{1}{2} \mathbf{a}_1 - x_4 \mathbf{a}_2 - (x_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}$	(12e)	S I
\mathbf{B}_{17}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(12e)	S I
\mathbf{B}_{18}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(12e)	S I
\mathbf{B}_{19}	$= x_4 \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + ax_4 \hat{\mathbf{z}}$	(12e)	S I
\mathbf{B}_{20}	$= -x_4 \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - ax_4 \hat{\mathbf{z}}$	(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}	$= -(y_5 + z_5) \mathbf{a}_1 + (x_5 - z_5) \mathbf{a}_2 + (x_5 - y_5) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}}$	(24f)	Hf III
\mathbf{B}_{25}	$= (x_5 + y_5) \mathbf{a}_1 + (y_5 + z_5) \mathbf{a}_2 + (x_5 + z_5) \mathbf{a}_3$	$=$	$az_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}}$	(24f)	Hf III

$$\begin{aligned}
\mathbf{B}_{26} &= - (x_5 + y_5) \mathbf{a}_1 - (y_5 - z_5) \mathbf{a}_2 - (x_5 - z_5) \mathbf{a}_3 &= & az_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}} & (24f) & \text{Hf III} \\
\mathbf{B}_{27} &= - (x_5 - y_5) \mathbf{a}_1 + (y_5 - z_5) \mathbf{a}_2 - (x_5 + z_5) \mathbf{a}_3 &= & -az_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}} & (24f) & \text{Hf III} \\
\mathbf{B}_{28} &= (x_5 - y_5) \mathbf{a}_1 - (y_5 + z_5) \mathbf{a}_2 + (x_5 - z_5) \mathbf{a}_3 &= & -az_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}} & (24f) & \text{Hf III} \\
\mathbf{B}_{29} &= (x_5 + z_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + (y_5 + z_5) \mathbf{a}_3 &= & ay_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}} & (24f) & \text{Hf III} \\
\mathbf{B}_{30} &= - (x_5 - z_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 - (y_5 - z_5) \mathbf{a}_3 &= & -ay_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}} & (24f) & \text{Hf III} \\
\mathbf{B}_{31} &= - (x_5 + z_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + (y_5 - z_5) \mathbf{a}_3 &= & ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}} & (24f) & \text{Hf III} \\
\mathbf{B}_{32} &= (x_5 - z_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 - (y_5 + z_5) \mathbf{a}_3 &= & -ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}} & (24f) & \text{Hf III}
\end{aligned}$$

References

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