

Ta₂₁Te₁₃ Structure:

A21B13_hP136_183_abc3d6e2f_2ab3d5e-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://aflow.org/p/7BEE>

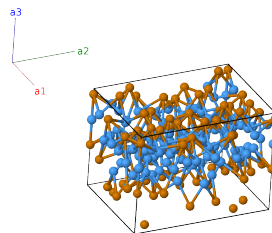
https://aflow.org/p/A21B13_hP136_183_abc3d6e2f_2ab3d5e-001

Prototype	Ta ₂₁ Te ₁₃
AFLOW prototype label	A21B13_hP136_183_abc3d6e2f_2ab3d5e-001
ICSD	91811
Pearson symbol	hP136
Space group number	183
Space group symbol	<i>P6mm</i>
AFLOW prototype command	<pre>aflow --proto=A21B13_hP136_183_abc3d6e2f_2ab3d5e-001 --params=a,c/a,z1,z2,z3,z4,z5,z6,x7,z7,x8,z8,x9,z9,x10,z10,x11,z11,x12,z12,x13, z13,x14,z14,x15,z15,x16,z16,x17,z17,x18,z18,x19,z19,x20,z20,x21,z21,x22,z22,x23,z23,x24, y24,z24,x25,y25,z25</pre>

- This is a hexagonal *approximate* of the quasicrystal dodecagonal tantalum telluride (dd-Ta_{1.6}Te) structure. It may be useful as a starting point for first-principles calculations.
- Space group *P6mm* #183 does not specify the origin of the *z*-axis. We use the values of (Conrad, 2000). (Villars, 2006) sets $z_2 = 0$ for the Te-I site.

Hexagonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
B₁ =	$z_1 \mathbf{a}_3$	=	$cz_1 \hat{\mathbf{z}}$	(1a)	Ta I
B₂ =	$z_2 \mathbf{a}_3$	=	$cz_2 \hat{\mathbf{z}}$	(1a)	Te I
B₃ =	$z_3 \mathbf{a}_3$	=	$cz_3 \hat{\mathbf{z}}$	(1a)	Te II
B₄ =	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2b)	Ta II
B₅ =	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2b)	Ta II
B₆ =	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(2b)	Te III

$$\mathbf{B}_{127} = -(x_{25} - y_{25}) \mathbf{a}_1 - x_{25} \mathbf{a}_2 + z_{25} \mathbf{a}_3 = -\frac{1}{2}a(2x_{25} - y_{25}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{25} \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}} \quad (12f) \quad \text{Ta XIV}$$

$$\mathbf{B}_{128} = -x_{25} \mathbf{a}_1 - y_{25} \mathbf{a}_2 + z_{25} \mathbf{a}_3 = -\frac{1}{2}a(x_{25} + y_{25}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{25} - y_{25}) \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}} \quad (12f) \quad \text{Ta XIV}$$

$$\mathbf{B}_{129} = y_{25} \mathbf{a}_1 - (x_{25} - y_{25}) \mathbf{a}_2 + z_{25} \mathbf{a}_3 = \frac{1}{2}a(-x_{25} + 2y_{25}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{25} \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}} \quad (12f) \quad \text{Ta XIV}$$

$$\mathbf{B}_{130} = (x_{25} - y_{25}) \mathbf{a}_1 + x_{25} \mathbf{a}_2 + z_{25} \mathbf{a}_3 = \frac{1}{2}a(2x_{25} - y_{25}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{25} \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}} \quad (12f) \quad \text{Ta XIV}$$

$$\mathbf{B}_{131} = -y_{25} \mathbf{a}_1 - x_{25} \mathbf{a}_2 + z_{25} \mathbf{a}_3 = -\frac{1}{2}a(x_{25} + y_{25}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{25} - y_{25}) \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}} \quad (12f) \quad \text{Ta XIV}$$

$$\mathbf{B}_{132} = -(x_{25} - y_{25}) \mathbf{a}_1 + y_{25} \mathbf{a}_2 + z_{25} \mathbf{a}_3 = \frac{1}{2}a(-x_{25} + 2y_{25}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{25} \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}} \quad (12f) \quad \text{Ta XIV}$$

$$\mathbf{B}_{133} = x_{25} \mathbf{a}_1 + (x_{25} - y_{25}) \mathbf{a}_2 + z_{25} \mathbf{a}_3 = \frac{1}{2}a(2x_{25} - y_{25}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{25} \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}} \quad (12f) \quad \text{Ta XIV}$$

$$\mathbf{B}_{134} = y_{25} \mathbf{a}_1 + x_{25} \mathbf{a}_2 + z_{25} \mathbf{a}_3 = \frac{1}{2}a(x_{25} + y_{25}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{25} - y_{25}) \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}} \quad (12f) \quad \text{Ta XIV}$$

$$\mathbf{B}_{135} = (x_{25} - y_{25}) \mathbf{a}_1 - y_{25} \mathbf{a}_2 + z_{25} \mathbf{a}_3 = \frac{1}{2}a(x_{25} - 2y_{25}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{25} \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}} \quad (12f) \quad \text{Ta XIV}$$

$$\mathbf{B}_{136} = -x_{25} \mathbf{a}_1 - (x_{25} - y_{25}) \mathbf{a}_2 + z_{25} \mathbf{a}_3 = -\frac{1}{2}a(2x_{25} - y_{25}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{25} \hat{\mathbf{y}} + cz_{25} \hat{\mathbf{z}} \quad (12f) \quad \text{Ta XIV}$$

References

- [1] M. Conrad, F. Krumeich, C. Reich, and B. Harbrecht, *Hexagonal approximants of a dodecagonal tantalum telluride – the crystal structure of $Ta_{21}Te_{13}$* , msea **294-296**, 37–40 (2000), doi:10.1016/S0921-5093(00)01150-3.

Found in

- [1] P. Villars, K. Cenzual, J. Daams, R. Gladyshevskii, O. Shcherban, V. Dubenskyy, N. Melnichenko-Koblyuk, O. Pavlyuk, I. Savesyuk, S. Stoiko, and L. Sysa, *Landolt-Börnstein - Group III Condensed Matter 43A4* (Springer-Verlag, Berlin Heidelberg, 2006), chap. Structure Types. Part 4: Space Groups (189) P-62m - (174) P-6. $Ta_{21}Te_{13}$, doi:10.1007/10920527_353.

● Ta
● Te

