

Ta₂₁Te₁₃ Structure:

A21B13_hP136_183_abc3d6e2f_2ab3d5e-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/7BEE>

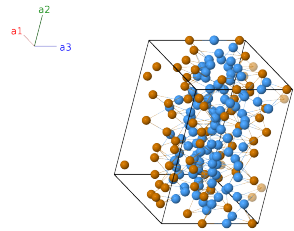
https://aflow.org/prototype-encyclopedia/A21B13_hP136_183_abc3d6e2f_2ab3d5e-001

Prototype	Ta ₂₁ Te ₁₃
AFLOW prototype label	A21B13_hP136_183_abc3d6e2f_2ab3d5e-001
ICSD	91811
CCDC	1651334
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
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(1a)	Ta I
$\mathbf{B}_2$	$= z_2 \mathbf{a}_3$	$=$	$c z_2 \hat{\mathbf{z}}$	(1a)	Te I

B ₈₅	=	-2x ₁₉ a ₁ - x ₁₉ a ₂ + z ₁₉ a ₃	=	$-\frac{3}{2}ax_{19}\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_{19}\hat{\mathbf{y}}+cz_{19}\hat{\mathbf{z}}$	(6e)	Te VII
B ₈₆	=	-x ₁₉ a ₁ + x ₁₉ a ₂ + z ₁₉ a ₃	=	$\sqrt{3}ax_{19}\hat{\mathbf{y}}+cz_{19}\hat{\mathbf{z}}$	(6e)	Te VII
B ₈₇	=	-x ₁₉ a ₁ - 2x ₁₉ a ₂ + z ₁₉ a ₃	=	$-\frac{3}{2}ax_{19}\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_{19}\hat{\mathbf{y}}+cz_{19}\hat{\mathbf{z}}$	(6e)	Te VII
B ₈₈	=	2x ₁₉ a ₁ + x ₁₉ a ₂ + z ₁₉ a ₃	=	$\frac{3}{2}ax_{19}\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_{19}\hat{\mathbf{y}}+cz_{19}\hat{\mathbf{z}}$	(6e)	Te VII
B ₈₉	=	x ₂₀ a ₁ - x ₂₀ a ₂ + z ₂₀ a ₃	=	$-\sqrt{3}ax_{20}\hat{\mathbf{y}}+cz_{20}\hat{\mathbf{z}}$	(6e)	Te VIII
B ₉₀	=	x ₂₀ a ₁ + 2x ₂₀ a ₂ + z ₂₀ a ₃	=	$\frac{3}{2}ax_{20}\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_{20}\hat{\mathbf{y}}+cz_{20}\hat{\mathbf{z}}$	(6e)	Te VIII
B ₉₁	=	-2x ₂₀ a ₁ - x ₂₀ a ₂ + z ₂₀ a ₃	=	$-\frac{3}{2}ax_{20}\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_{20}\hat{\mathbf{y}}+cz_{20}\hat{\mathbf{z}}$	(6e)	Te VIII
B ₉₂	=	-x ₂₀ a ₁ + x ₂₀ a ₂ + z ₂₀ a ₃	=	$\sqrt{3}ax_{20}\hat{\mathbf{y}}+cz_{20}\hat{\mathbf{z}}$	(6e)	Te VIII
B ₉₃	=	-x ₂₀ a ₁ - 2x ₂₀ a ₂ + z ₂₀ a ₃	=	$-\frac{3}{2}ax_{20}\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_{20}\hat{\mathbf{y}}+cz_{20}\hat{\mathbf{z}}$	(6e)	Te VIII
B ₉₄	=	2x ₂₀ a ₁ + x ₂₀ a ₂ + z ₂₀ a ₃	=	$\frac{3}{2}ax_{20}\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_{20}\hat{\mathbf{y}}+cz_{20}\hat{\mathbf{z}}$	(6e)	Te VIII
B ₉₅	=	x ₂₁ a ₁ - x ₂₁ a ₂ + z ₂₁ a ₃	=	$-\sqrt{3}ax_{21}\hat{\mathbf{y}}+cz_{21}\hat{\mathbf{z}}$	(6e)	Te IX
B ₉₆	=	x ₂₁ a ₁ + 2x ₂₁ a ₂ + z ₂₁ a ₃	=	$\frac{3}{2}ax_{21}\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_{21}\hat{\mathbf{y}}+cz_{21}\hat{\mathbf{z}}$	(6e)	Te IX
B ₉₇	=	-2x ₂₁ a ₁ - x ₂₁ a ₂ + z ₂₁ a ₃	=	$-\frac{3}{2}ax_{21}\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_{21}\hat{\mathbf{y}}+cz_{21}\hat{\mathbf{z}}$	(6e)	Te IX
B ₉₈	=	-x ₂₁ a ₁ + x ₂₁ a ₂ + z ₂₁ a ₃	=	$\sqrt{3}ax_{21}\hat{\mathbf{y}}+cz_{21}\hat{\mathbf{z}}$	(6e)	Te IX
B ₉₉	=	-x ₂₁ a ₁ - 2x ₂₁ a ₂ + z ₂₁ a ₃	=	$-\frac{3}{2}ax_{21}\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_{21}\hat{\mathbf{y}}+cz_{21}\hat{\mathbf{z}}$	(6e)	Te IX
B ₁₀₀	=	2x ₂₁ a ₁ + x ₂₁ a ₂ + z ₂₁ a ₃	=	$\frac{3}{2}ax_{21}\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_{21}\hat{\mathbf{y}}+cz_{21}\hat{\mathbf{z}}$	(6e)	Te IX
B ₁₀₁	=	x ₂₂ a ₁ - x ₂₂ a ₂ + z ₂₂ a ₃	=	$-\sqrt{3}ax_{22}\hat{\mathbf{y}}+cz_{22}\hat{\mathbf{z}}$	(6e)	Te X
B ₁₀₂	=	x ₂₂ a ₁ + 2x ₂₂ a ₂ + z ₂₂ a ₃	=	$\frac{3}{2}ax_{22}\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_{22}\hat{\mathbf{y}}+cz_{22}\hat{\mathbf{z}}$	(6e)	Te X
B ₁₀₃	=	-2x ₂₂ a ₁ - x ₂₂ a ₂ + z ₂₂ a ₃	=	$-\frac{3}{2}ax_{22}\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_{22}\hat{\mathbf{y}}+cz_{22}\hat{\mathbf{z}}$	(6e)	Te X
B ₁₀₄	=	-x ₂₂ a ₁ + x ₂₂ a ₂ + z ₂₂ a ₃	=	$\sqrt{3}ax_{22}\hat{\mathbf{y}}+cz_{22}\hat{\mathbf{z}}$	(6e)	Te X
B ₁₀₅	=	-x ₂₂ a ₁ - 2x ₂₂ a ₂ + z ₂₂ a ₃	=	$-\frac{3}{2}ax_{22}\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_{22}\hat{\mathbf{y}}+cz_{22}\hat{\mathbf{z}}$	(6e)	Te X
B ₁₀₆	=	2x ₂₂ a ₁ + x ₂₂ a ₂ + z ₂₂ a ₃	=	$\frac{3}{2}ax_{22}\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_{22}\hat{\mathbf{y}}+cz_{22}\hat{\mathbf{z}}$	(6e)	Te X
B ₁₀₇	=	x ₂₃ a ₁ - x ₂₃ a ₂ + z ₂₃ a ₃	=	$-\sqrt{3}ax_{23}\hat{\mathbf{y}}+cz_{23}\hat{\mathbf{z}}$	(6e)	Te XI
B ₁₀₈	=	x ₂₃ a ₁ + 2x ₂₃ a ₂ + z ₂₃ a ₃	=	$\frac{3}{2}ax_{23}\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_{23}\hat{\mathbf{y}}+cz_{23}\hat{\mathbf{z}}$	(6e)	Te XI
B ₁₀₉	=	-2x ₂₃ a ₁ - x ₂₃ a ₂ + z ₂₃ a ₃	=	$-\frac{3}{2}ax_{23}\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_{23}\hat{\mathbf{y}}+cz_{23}\hat{\mathbf{z}}$ </		

$$\begin{aligned}
\mathbf{B}_{123} &= (x_{24} - y_{24}) \mathbf{a}_1 - y_{24} \mathbf{a}_2 + z_{24} \mathbf{a}_3 = \frac{1}{2}a(x_{24} - 2y_{24}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{24} \hat{\mathbf{y}} + cz_{24} \hat{\mathbf{z}} & (12f) & \text{Ta XIII} \\
\mathbf{B}_{124} &= -x_{24} \mathbf{a}_1 - (x_{24} - y_{24}) \mathbf{a}_2 + z_{24} \mathbf{a}_3 = -\frac{1}{2}a(2x_{24} - y_{24}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{24} \hat{\mathbf{y}} + cz_{24} \hat{\mathbf{z}} & (12f) & \text{Ta XIII} \\
\mathbf{B}_{125} &= 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}} & (12f) & \text{Ta XIV} \\
\mathbf{B}_{126} &= -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}} & (12f) & \text{Ta XIV} \\
\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}} & (12f) & \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}} & (12f) & \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}} & (12f) & \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}} & (12f) & \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}} & (12f) & \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}} & (12f) & \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}} & (12f) & \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}} & (12f) & \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}} & (12f) & \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}} & (12f) & \text{Ta XIV}
\end{aligned}$$

References

- [1] M. Conrad, F. Krumeich, C. Reich, and B. Harbrecht, *Hexagonal approximants of a dodecagonal tantalum telluride – the crystal structure of Ta₂₁Te₁₃*, msea **294-296**, 37–40 (2000), doi:10.1016/S0921-5093(00)01150-3.

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- [1] P. Villars, K. Cenzual, J. Daams, R. Gladyshevskii, O. Shcherban, V. Dubenskiy, 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. Ta₂₁Te₁₃, doi:10.1007/10920527_353.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.

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