

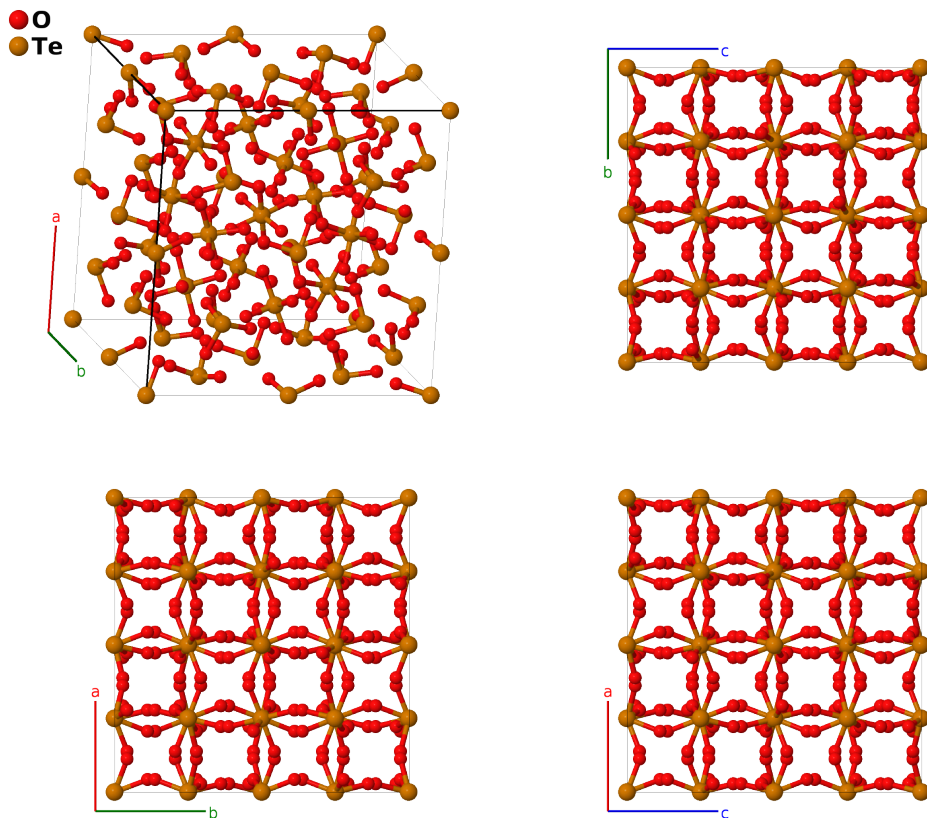
Te[OH]₆ Structure (*Obsolete*): A6B_cF224_228_h_c-001

This structure originally had the label A6B_cF224_228_h_c. Calls to that address will be redirected here.

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<https://afLOW.org/p/MSL9>

https://afLOW.org/p/A6B_cF224_228_h_c-001



Prototype	H ₆ O ₆ Te
AFLOW prototype label	A6B_cF224_228_h_c-001
ICSD	none
Pearson symbol	cF224
Space group number	228
Space group symbol	$Fd\bar{3}c$
AFLOW prototype command	<code>afLOW --proto=A6B_cF224_228_h_c-001 --params=a, x₂, y₂, z₂</code>

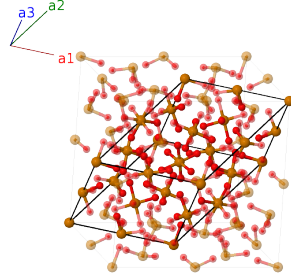
- (Kirkpatrick, 1926) did not find the locations of the hydrogen atoms. When these were located by (Mullica, 1980) it was found that the true structure is in space group $F4_132$ #210.

Face-centered Cubic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(32c)	Te I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}}$	(32c)	Te I
\mathbf{B}_3	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{z}}$	(32c)	Te I
\mathbf{B}_4	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(32c)	Te I
\mathbf{B}_5	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(32c)	Te I
\mathbf{B}_6	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(32c)	Te I
\mathbf{B}_7	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(32c)	Te I
\mathbf{B}_8	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(32c)	Te I
\mathbf{B}_9	$(-x_2 + y_2 + z_2) \mathbf{a}_1 +$ $(x_2 - y_2 + z_2) \mathbf{a}_2 +$ $(x_2 + y_2 - z_2) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}}$	(192h)	O I
\mathbf{B}_{10}	$(x_2 - y_2 + z_2) \mathbf{a}_1 +$ $(-x_2 + y_2 + z_2) \mathbf{a}_2 -$ $(x_2 + y_2 + z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{4}) \hat{\mathbf{x}} - a(y_2 - \frac{1}{4}) \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}}$	(192h)	O I
\mathbf{B}_{11}	$(x_2 + y_2 - z_2) \mathbf{a}_1 -$ $(x_2 + y_2 + z_2 - \frac{1}{2}) \mathbf{a}_2 +$ $(-x_2 + y_2 + z_2) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{4}) \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} - a(z_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(192h)	O I
\mathbf{B}_{12}	$-(x_2 + y_2 + z_2 - \frac{1}{2}) \mathbf{a}_1 +$ $(x_2 + y_2 - z_2) \mathbf{a}_2 +$ $(x_2 - y_2 + z_2) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - a(y_2 - \frac{1}{4}) \hat{\mathbf{y}} - a(z_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(192h)	O I
\mathbf{B}_{13}	$(x_2 + y_2 - z_2) \mathbf{a}_1 +$ $(-x_2 + y_2 + z_2) \mathbf{a}_2 +$ $(x_2 - y_2 + z_2) \mathbf{a}_3$	$=$	$az_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ay_2 \hat{\mathbf{z}}$	(192h)	O I
\mathbf{B}_{14}	$-(x_2 + y_2 + z_2 - \frac{1}{2}) \mathbf{a}_1 +$ $(x_2 - y_2 + z_2) \mathbf{a}_2 +$ $(-x_2 + y_2 + z_2) \mathbf{a}_3$	$=$	$az_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{4}) \hat{\mathbf{y}} - a(y_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(192h)	O I
\mathbf{B}_{15}	$(-x_2 + y_2 + z_2) \mathbf{a}_1 +$ $(x_2 + y_2 - z_2) \mathbf{a}_2 -$ $(x_2 + y_2 + z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(z_2 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{4}) \hat{\mathbf{y}} + ay_2 \hat{\mathbf{z}}$	(192h)	O I
\mathbf{B}_{16}	$(x_2 - y_2 + z_2) \mathbf{a}_1 -$ $(x_2 + y_2 + z_2 - \frac{1}{2}) \mathbf{a}_2 +$ $(x_2 + y_2 - z_2) \mathbf{a}_3$	$=$	$-a(z_2 - \frac{1}{4}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - a(y_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(192h)	O I

$$\begin{aligned}
\mathbf{B}_{50} &= \begin{aligned} &-(x_2 + y_2 + z_2) \mathbf{a}_1 + \\ &(x_2 - y_2 + z_2 + \frac{1}{2}) \mathbf{a}_2 + \\ &(x_2 + y_2 - z_2 + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(z_2 - \frac{1}{4}) \hat{\mathbf{y}} - a(y_2 - \frac{1}{4}) \hat{\mathbf{z}} &(192h) & \text{O I} \\
\mathbf{B}_{51} &= \begin{aligned} &(-x_2 + y_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 + \\ &(x_2 + y_2 - z_2 + \frac{1}{2}) \mathbf{a}_2 + \\ &(x_2 - y_2 + z_2 + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + a(z_2 + \frac{1}{2}) \hat{\mathbf{y}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{z}} &(192h) & \text{O I} \\
\mathbf{B}_{52} &= \begin{aligned} &(x_2 - y_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 - \\ &(x_2 + y_2 + z_2) \mathbf{a}_2 + \\ &(-x_2 + y_2 + z_2 + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= -a(x_2 - \frac{1}{4}) \hat{\mathbf{x}} + a(z_2 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_2 - \frac{1}{4}) \hat{\mathbf{z}} &(192h) & \text{O I} \\
\mathbf{B}_{53} &= \begin{aligned} &(x_2 - y_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 + \\ &(x_2 + y_2 - z_2 + \frac{1}{2}) \mathbf{a}_2 - \\ &(x_2 + y_2 + z_2) \mathbf{a}_3 \end{aligned} &= -a(z_2 - \frac{1}{4}) \hat{\mathbf{x}} - a(y_2 - \frac{1}{4}) \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}} &(192h) & \text{O I} \\
\mathbf{B}_{54} &= \begin{aligned} &(-x_2 + y_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 - \\ &(x_2 + y_2 + z_2) \mathbf{a}_2 + \\ &(x_2 + y_2 - z_2 + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= -a(z_2 - \frac{1}{4}) \hat{\mathbf{x}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_2 - \frac{1}{4}) \hat{\mathbf{z}} &(192h) & \text{O I} \\
\mathbf{B}_{55} &= \begin{aligned} &-(x_2 + y_2 + z_2) \mathbf{a}_1 + \\ &(-x_2 + y_2 + z_2 + \frac{1}{2}) \mathbf{a}_2 + \\ &(x_2 - y_2 + z_2 + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= a(z_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_2 - \frac{1}{4}) \hat{\mathbf{y}} - a(x_2 - \frac{1}{4}) \hat{\mathbf{z}} &(192h) & \text{O I} \\
\mathbf{B}_{56} &= \begin{aligned} &(x_2 + y_2 - z_2 + \frac{1}{2}) \mathbf{a}_1 + \\ &(x_2 - y_2 + z_2 + \frac{1}{2}) \mathbf{a}_2 + \\ &(-x_2 + y_2 + z_2 + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= a(z_2 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}} &(192h) & \text{O I}
\end{aligned}$$

References

- [1] L. M. Kirkpatrick and L. Pauling, *Über die Kristallstruktur der kubischen Tellursäure*, Z. Krystallogr. **63**, 502–506 (1926), doi:10.1524/zkri.1926.63.1.502.
- [2] D. F. Mullica, J. D. Korp, W. O. Milligan, G. W. Beall, and I. Bernal, *Neutron structural refinement of cubic orthotelluric acid*, Acta Crystallogr. Sect. B **36**, 2565–2570 (1980), doi:10.1107/S0567740880009454.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.