

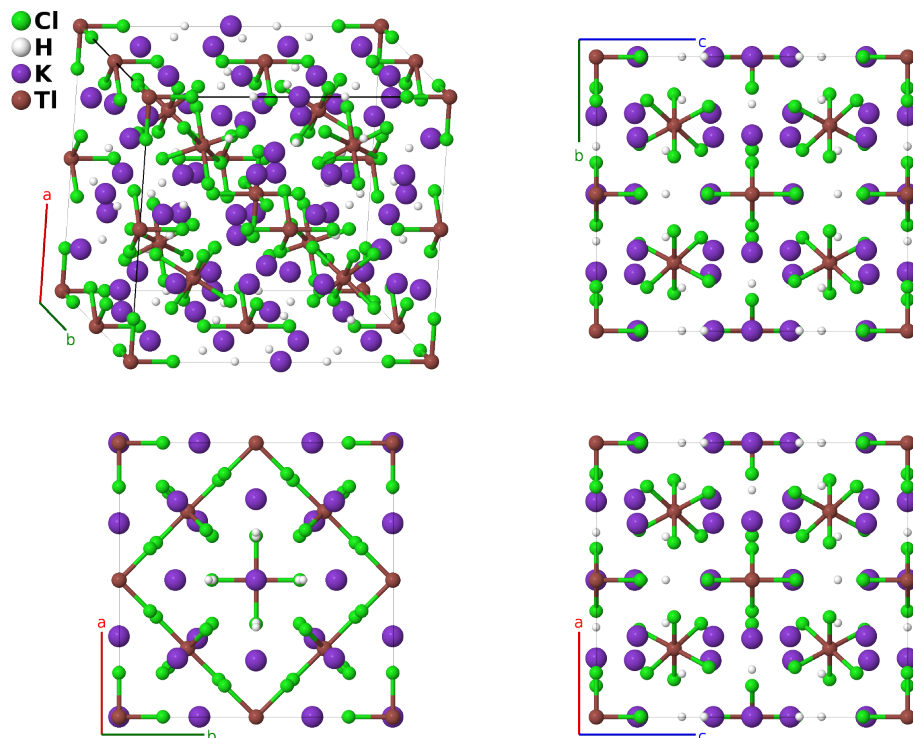
$K_3TiCl_6 \cdot 2H_2O$ ($J3_1$) Structure: A6B2C3D_tI168_139_egikl2m_ejn_bh2n_acf-001

This structure originally had the label A6B2C3D_tI168_139_egikl2m_ejn_bh2n_acf. Calls to that address will be redirected here.

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<https://aflow.org/p/8AAX>

https://aflow.org/p/A6B2C3D_tI168_139_egikl2m_ejn_bh2n_acf-001

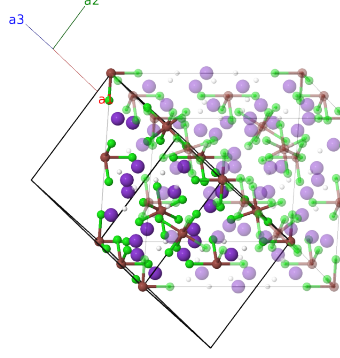


Prototype	$Cl_6(H_2O)_2K_3Ti$
AFLOW prototype label	A6B2C3D_tI168_139_egikl2m_ejn_bh2n_acf-001
<i>Strukturbericht</i> designation	$J3_1$
ICSD	31681
Pearson symbol	tI168
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	<pre>aflow --proto=A6B2C3D_tI168_139_egikl2m_ejn_bh2n_acf-001 --params=a, c/a, z4, z5, z7, x8, x9, x10, x11, x12, y12, x13, z13, x14, z14, y15, z15, y16, z16, y17, z17</pre>

- The positions of the hydrogen atoms in the water molecules were not determined, so we only provide the positions of the oxygen atoms (labeled as H_2O).

Body-centered Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(2a)	Tl I
\mathbf{B}_2	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{2}c\hat{\mathbf{z}}$	(2b)	K I
\mathbf{B}_3	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{y}}$	(4c)	Tl II
\mathbf{B}_4	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}}$	(4c)	Tl II
\mathbf{B}_5	$z_4\mathbf{a}_1 + z_4\mathbf{a}_2$	$=$	$cz_4\hat{\mathbf{z}}$	(4e)	Cl I
\mathbf{B}_6	$-z_4\mathbf{a}_1 - z_4\mathbf{a}_2$	$=$	$-cz_4\hat{\mathbf{z}}$	(4e)	Cl I
\mathbf{B}_7	$z_5\mathbf{a}_1 + z_5\mathbf{a}_2$	$=$	$cz_5\hat{\mathbf{z}}$	(4e)	H I
\mathbf{B}_8	$-z_5\mathbf{a}_1 - z_5\mathbf{a}_2$	$=$	$-cz_5\hat{\mathbf{z}}$	(4e)	H I
\mathbf{B}_9	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(8f)	Tl III
\mathbf{B}_{10}	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - \frac{1}{4}c\hat{\mathbf{z}}$	(8f)	Tl III
\mathbf{B}_{11}	$\frac{1}{2}\mathbf{a}_1$	$=$	$-\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(8f)	Tl III
\mathbf{B}_{12}	$\frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(8f)	Tl III
\mathbf{B}_{13}	$(z_7 + \frac{1}{2})\mathbf{a}_1 + z_7\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{y}} + cz_7\hat{\mathbf{z}}$	(8g)	Cl II
\mathbf{B}_{14}	$z_7\mathbf{a}_1 + (z_7 + \frac{1}{2})\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + cz_7\hat{\mathbf{z}}$	(8g)	Cl II
\mathbf{B}_{15}	$-(z_7 - \frac{1}{2})\mathbf{a}_1 - z_7\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{y}} - cz_7\hat{\mathbf{z}}$	(8g)	Cl II
\mathbf{B}_{16}	$-z_7\mathbf{a}_1 - (z_7 - \frac{1}{2})\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - cz_7\hat{\mathbf{z}}$	(8g)	Cl II
\mathbf{B}_{17}	$x_8\mathbf{a}_1 + x_8\mathbf{a}_2 + 2x_8\mathbf{a}_3$	$=$	$ax_8\hat{\mathbf{x}} + ax_8\hat{\mathbf{y}}$	(8h)	K II
\mathbf{B}_{18}	$-x_8\mathbf{a}_1 - x_8\mathbf{a}_2 - 2x_8\mathbf{a}_3$	$=$	$-ax_8\hat{\mathbf{x}} - ax_8\hat{\mathbf{y}}$	(8h)	K II
\mathbf{B}_{19}	$x_8\mathbf{a}_1 - x_8\mathbf{a}_2$	$=$	$-ax_8\hat{\mathbf{x}} + ax_8\hat{\mathbf{y}}$	(8h)	K II
\mathbf{B}_{20}	$-x_8\mathbf{a}_1 + x_8\mathbf{a}_2$	$=$	$ax_8\hat{\mathbf{x}} - ax_8\hat{\mathbf{y}}$	(8h)	K II
\mathbf{B}_{21}	$x_9\mathbf{a}_2 + x_9\mathbf{a}_3$	$=$	$ax_9\hat{\mathbf{x}}$	(8i)	Cl III
\mathbf{B}_{22}	$-x_9\mathbf{a}_2 - x_9\mathbf{a}_3$	$=$	$-ax_9\hat{\mathbf{x}}$	(8i)	Cl III
\mathbf{B}_{23}	$x_9\mathbf{a}_1 + x_9\mathbf{a}_3$	$=$	$ax_9\hat{\mathbf{y}}$	(8i)	Cl III
\mathbf{B}_{24}	$-x_9\mathbf{a}_1 - x_9\mathbf{a}_3$	$=$	$-ax_9\hat{\mathbf{y}}$	(8i)	Cl III
\mathbf{B}_{25}	$\frac{1}{2}\mathbf{a}_1 + x_{10}\mathbf{a}_2 + (x_{10} + \frac{1}{2})\mathbf{a}_3$	$=$	$ax_{10}\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}}$	(8j)	H II
\mathbf{B}_{26}	$\frac{1}{2}\mathbf{a}_1 - x_{10}\mathbf{a}_2 - (x_{10} - \frac{1}{2})\mathbf{a}_3$	$=$	$-ax_{10}\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}}$	(8j)	H II
\mathbf{B}_{27}	$x_{10}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + (x_{10} + \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + ax_{10}\hat{\mathbf{y}}$	(8j)	H II
\mathbf{B}_{28}	$-x_{10}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 - (x_{10} - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - ax_{10}\hat{\mathbf{y}}$	(8j)	H II

$$\begin{aligned}
\mathbf{B}_{59} &= \begin{pmatrix} (x_{14} - z_{14}) \mathbf{a}_1 + \\ (x_{14} - z_{14}) \mathbf{a}_2 + 2x_{14} \mathbf{a}_3 \end{pmatrix} = ax_{14} \hat{\mathbf{x}} + ax_{14} \hat{\mathbf{y}} - cz_{14} \hat{\mathbf{z}} & (16m) & \text{Cl VII} \\
\mathbf{B}_{60} &= \begin{pmatrix} -(x_{14} + z_{14}) \mathbf{a}_1 - \\ (x_{14} + z_{14}) \mathbf{a}_2 - 2x_{14} \mathbf{a}_3 \end{pmatrix} = -ax_{14} \hat{\mathbf{x}} - ax_{14} \hat{\mathbf{y}} - cz_{14} \hat{\mathbf{z}} & (16m) & \text{Cl VII} \\
\mathbf{B}_{61} &= (y_{15} + z_{15}) \mathbf{a}_1 + z_{15} \mathbf{a}_2 + y_{15} \mathbf{a}_3 = ay_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (16n) & \text{H III} \\
\mathbf{B}_{62} &= -(y_{15} - z_{15}) \mathbf{a}_1 + z_{15} \mathbf{a}_2 - y_{15} \mathbf{a}_3 = -ay_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (16n) & \text{H III} \\
\mathbf{B}_{63} &= z_{15} \mathbf{a}_1 - (y_{15} - z_{15}) \mathbf{a}_2 - y_{15} \mathbf{a}_3 = -ay_{15} \hat{\mathbf{x}} + cz_{15} \hat{\mathbf{z}} & (16n) & \text{H III} \\
\mathbf{B}_{64} &= z_{15} \mathbf{a}_1 + (y_{15} + z_{15}) \mathbf{a}_2 + y_{15} \mathbf{a}_3 = ay_{15} \hat{\mathbf{x}} + cz_{15} \hat{\mathbf{z}} & (16n) & \text{H III} \\
\mathbf{B}_{65} &= (y_{15} - z_{15}) \mathbf{a}_1 - z_{15} \mathbf{a}_2 + y_{15} \mathbf{a}_3 = ay_{15} \hat{\mathbf{y}} - cz_{15} \hat{\mathbf{z}} & (16n) & \text{H III} \\
\mathbf{B}_{66} &= -(y_{15} + z_{15}) \mathbf{a}_1 - z_{15} \mathbf{a}_2 - y_{15} \mathbf{a}_3 = -ay_{15} \hat{\mathbf{y}} - cz_{15} \hat{\mathbf{z}} & (16n) & \text{H III} \\
\mathbf{B}_{67} &= -z_{15} \mathbf{a}_1 + (y_{15} - z_{15}) \mathbf{a}_2 + y_{15} \mathbf{a}_3 = ay_{15} \hat{\mathbf{x}} - cz_{15} \hat{\mathbf{z}} & (16n) & \text{H III} \\
\mathbf{B}_{68} &= -z_{15} \mathbf{a}_1 - (y_{15} + z_{15}) \mathbf{a}_2 - y_{15} \mathbf{a}_3 = -ay_{15} \hat{\mathbf{x}} - cz_{15} \hat{\mathbf{z}} & (16n) & \text{H III} \\
\mathbf{B}_{69} &= (y_{16} + z_{16}) \mathbf{a}_1 + z_{16} \mathbf{a}_2 + y_{16} \mathbf{a}_3 = ay_{16} \hat{\mathbf{y}} + cz_{16} \hat{\mathbf{z}} & (16n) & \text{K III} \\
\mathbf{B}_{70} &= -(y_{16} - z_{16}) \mathbf{a}_1 + z_{16} \mathbf{a}_2 - y_{16} \mathbf{a}_3 = -ay_{16} \hat{\mathbf{y}} + cz_{16} \hat{\mathbf{z}} & (16n) & \text{K III} \\
\mathbf{B}_{71} &= z_{16} \mathbf{a}_1 - (y_{16} - z_{16}) \mathbf{a}_2 - y_{16} \mathbf{a}_3 = -ay_{16} \hat{\mathbf{x}} + cz_{16} \hat{\mathbf{z}} & (16n) & \text{K III} \\
\mathbf{B}_{72} &= z_{16} \mathbf{a}_1 + (y_{16} + z_{16}) \mathbf{a}_2 + y_{16} \mathbf{a}_3 = ay_{16} \hat{\mathbf{x}} + cz_{16} \hat{\mathbf{z}} & (16n) & \text{K III} \\
\mathbf{B}_{73} &= (y_{16} - z_{16}) \mathbf{a}_1 - z_{16} \mathbf{a}_2 + y_{16} \mathbf{a}_3 = ay_{16} \hat{\mathbf{y}} - cz_{16} \hat{\mathbf{z}} & (16n) & \text{K III} \\
\mathbf{B}_{74} &= -(y_{16} + z_{16}) \mathbf{a}_1 - z_{16} \mathbf{a}_2 - y_{16} \mathbf{a}_3 = -ay_{16} \hat{\mathbf{y}} - cz_{16} \hat{\mathbf{z}} & (16n) & \text{K III} \\
\mathbf{B}_{75} &= -z_{16} \mathbf{a}_1 + (y_{16} - z_{16}) \mathbf{a}_2 + y_{16} \mathbf{a}_3 = ay_{16} \hat{\mathbf{x}} - cz_{16} \hat{\mathbf{z}} & (16n) & \text{K III} \\
\mathbf{B}_{76} &= -z_{16} \mathbf{a}_1 - (y_{16} + z_{16}) \mathbf{a}_2 - y_{16} \mathbf{a}_3 = -ay_{16} \hat{\mathbf{x}} - cz_{16} \hat{\mathbf{z}} & (16n) & \text{K III} \\
\mathbf{B}_{77} &= (y_{17} + z_{17}) \mathbf{a}_1 + z_{17} \mathbf{a}_2 + y_{17} \mathbf{a}_3 = ay_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}} & (16n) & \text{K IV} \\
\mathbf{B}_{78} &= -(y_{17} - z_{17}) \mathbf{a}_1 + z_{17} \mathbf{a}_2 - y_{17} \mathbf{a}_3 = -ay_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}} & (16n) & \text{K IV} \\
\mathbf{B}_{79} &= z_{17} \mathbf{a}_1 - (y_{17} - z_{17}) \mathbf{a}_2 - y_{17} \mathbf{a}_3 = -ay_{17} \hat{\mathbf{x}} + cz_{17} \hat{\mathbf{z}} & (16n) & \text{K IV} \\
\mathbf{B}_{80} &= z_{17} \mathbf{a}_1 + (y_{17} + z_{17}) \mathbf{a}_2 + y_{17} \mathbf{a}_3 = ay_{17} \hat{\mathbf{x}} + cz_{17} \hat{\mathbf{z}} & (16n) & \text{K IV} \\
\mathbf{B}_{81} &= (y_{17} - z_{17}) \mathbf{a}_1 - z_{17} \mathbf{a}_2 + y_{17} \mathbf{a}_3 = ay_{17} \hat{\mathbf{y}} - cz_{17} \hat{\mathbf{z}} & (16n) & \text{K IV} \\
\mathbf{B}_{82} &= -(y_{17} + z_{17}) \mathbf{a}_1 - z_{17} \mathbf{a}_2 - y_{17} \mathbf{a}_3 = -ay_{17} \hat{\mathbf{y}} - cz_{17} \hat{\mathbf{z}} & (16n) & \text{K IV} \\
\mathbf{B}_{83} &= -z_{17} \mathbf{a}_1 + (y_{17} - z_{17}) \mathbf{a}_2 + y_{17} \mathbf{a}_3 = ay_{17} \hat{\mathbf{x}} - cz_{17} \hat{\mathbf{z}} & (16n) & \text{K IV} \\
\mathbf{B}_{84} &= -z_{17} \mathbf{a}_1 - (y_{17} + z_{17}) \mathbf{a}_2 - y_{17} \mathbf{a}_3 = -ay_{17} \hat{\mathbf{x}} - cz_{17} \hat{\mathbf{z}} & (16n) & \text{K IV}
\end{aligned}$$

References

- [1] J. L. Hoard and L. Goldstein, *The Structure of Potassium Hexachlorothalliate Dihydrate*, J. Chem. Phys. **3**, 645–649 (1935), doi:10.1063/1.1749568.

Found in

- [1] C. Gottfried and F. Schosberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).