

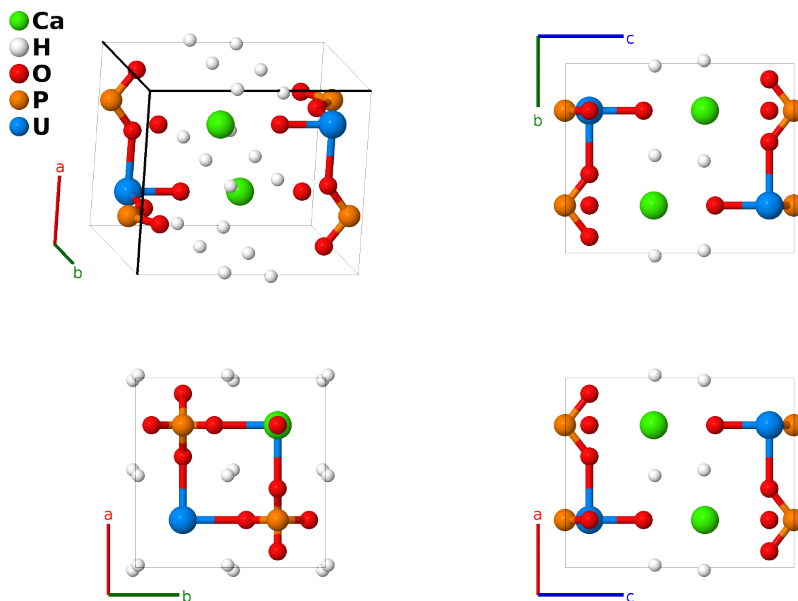
Meta-autunite (I) $[\text{Ca}(\text{UO}_2)_2(\text{PO}_4)_2 \cdot 6\text{H}_2\text{O}, H5_{10}]$ Structure: AB4C6DE_tP26_129_c_j_2ci_a_c-001

This structure originally had the label AB4C6DE_tP26_129_c_j_2ci_a_c. Calls to that address will be redirected here.

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

https://aflow.org/p/AB4C6DE_tP26_129_c_j_2ci_a_c-001



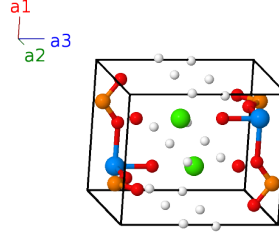
Prototype	$\text{Ca}(\text{H}_2\text{O})_6\text{O}_6\text{P}_2\text{U}_2$
AFLOW prototype label	AB4C6DE_tP26_129_c_j_2ci_a_c-001
<i>Strukturbericht</i> designation	$H5_{10}$
Mineral name	meta-autunite (I)
ICSD	none
Pearson symbol	tP26
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	<pre>aflow --proto=AB4C6DE_tP26_129_c_j_2ci_a_c-001 --params=a, c/a, z2, z3, z4, z5, y6, z6, x7, z7</pre>

- Autunite $\text{Ca}(\text{UO}_2)_2(\text{PO}_4)_2 \cdot n\text{H}_2\text{O}$, is found in three varieties: naturally occurring autunite, with $n \geq 10$, and meta-autunite (I), which is partially dehydrated, $6 \leq n < 10$. Further dehydration in the laboratory produces meta-autunite (II).
- The Calcium site is occupied 50% of the time, while 75% of the water sites are filled.

- (Beintema, 1938) proposed a structure for meta-autunite (I), which (Herrmann, 1941) designated $H5_{10}$. He did not locate the calcium and oxygen atoms nor the water molecules. This structure was improved by (Makarov, 1960), and we include it here as our prototype for $H5_{10}$. The Ca-I site is 50% occupied, while the H2O-I site is 75% occupied.

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(2a)	P I
\mathbf{B}_2	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(2a)	P I
\mathbf{B}_3	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2c)	Ca I
\mathbf{B}_4	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(2c)	Ca I
\mathbf{B}_5	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2c)	O I
\mathbf{B}_6	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(2c)	O I
\mathbf{B}_7	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2c)	O II
\mathbf{B}_8	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(2c)	O II
\mathbf{B}_9	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(2c)	U I
\mathbf{B}_{10}	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(2c)	U I
\mathbf{B}_{11}	$= \frac{1}{4} \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8i)	O III
\mathbf{B}_{12}	$= \frac{1}{4} \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8i)	O III
\mathbf{B}_{13}	$= -(y_6 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8i)	O III
\mathbf{B}_{14}	$= y_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8i)	O III
\mathbf{B}_{15}	$= \frac{3}{4} \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8i)	O III
\mathbf{B}_{16}	$= \frac{3}{4} \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8i)	O III
\mathbf{B}_{17}	$= (y_6 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$a(y_6 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8i)	O III
\mathbf{B}_{18}	$= -y_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8i)	O III
\mathbf{B}_{19}	$= x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8j)	H I
\mathbf{B}_{20}	$= -(x_7 - \frac{1}{2}) \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8j)	H I
\mathbf{B}_{21}	$= -(x_7 - \frac{1}{2}) \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8j)	H I
\mathbf{B}_{22}	$= x_7 \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8j)	H I
\mathbf{B}_{23}	$= -x_7 \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8j)	H I
\mathbf{B}_{24}	$= (x_7 + \frac{1}{2}) \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8j)	H I
\mathbf{B}_{25}	$= (x_7 + \frac{1}{2}) \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8j)	H I
\mathbf{B}_{26}	$= -x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8j)	H I

References

- [1] E. S. Makarov and V. I. Ivanov, *The crystal structure of meta-autunite, $Ca(UO_2)_2(PO_4)_2 \cdot 6H_2O$* , Doklady Akademii Nauk SSSR **132**, 601–603 (1960).
- [2] J. Beintema, *On the composition and the crystallography of autunite and the meta-autunites*, Rec. Trav. Chim. Pays-Bas **57**, 155–175 (1938), doi:10.1002/recl.19380570206.
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