$H5_9$ [Autunite $Ca(UO_2)_2(PO_4)_2 \cdot 10\frac{1}{2}H_2O$] Structure (*Obsolete*): AB2C2_tI10_139_a_d_e-003

This structure originally had the label `AB2C2_tI10_139_a_d_e`. Calls to that address will be redirected here.

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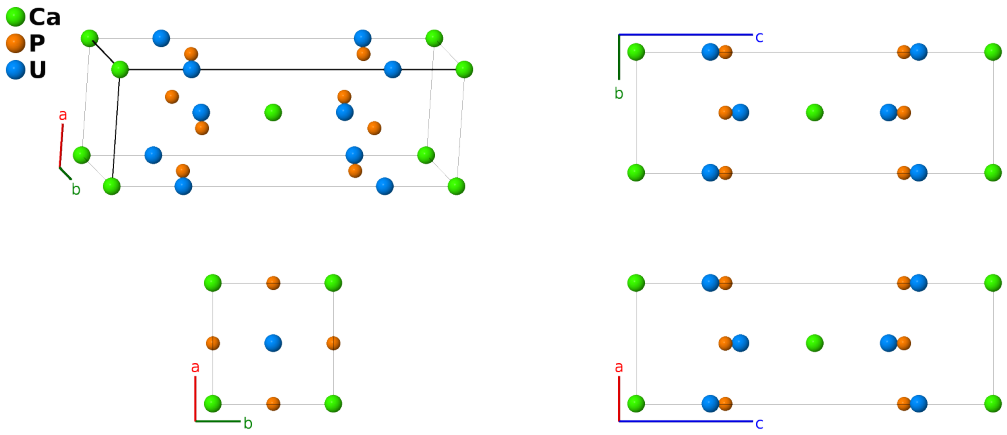
https://aflow.org/p/SC3Z

https://aflow.org/p/AB2C2_tI10_139_a_d_e-003



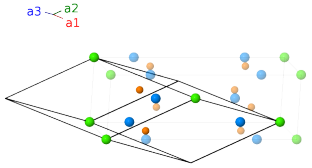
Prototype	$Ca(H_2O)_{10.5}(PO_4)_2(UO_2)_2$
AFLOW prototype label	AB2C2_tI10_139_a_d_e-003
***Strukturbericht* designation**	$H5_9$
Mineral name	autunite
ICSD	33193
Pearson symbol	tI10
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=AB2C2_tI10_139_a_d_e-003 --params=`$a, c/a, z_3$

- Autunite $Ca(UO_2)_2(PO_4)_2 \cdot nH_2O$, is found in three varieties:
- Naturally occurring Autunite, with $n \geq 10$,
- Partially dehydrated meta-autunite (I) ($6 \leq n \leq 10$).
- Further dehydration in the laboratory produces meta-autunite (II).
- (Beintema, 1938) proposed this structure for autunite, which (Herrmann, 1941) designated $H5_9$. This original tetragonal structure did not locate the oxygen atoms or the water molecules, although the ICSD entry does list atomic positions for the oxygen atoms which are not obviously obtained from the paper. Later determinations of this structure (Locock, 2003) located all the atoms in the crystal for $n = 11$, and found the structure to be orthorhombic.

- This form of autonite and Li_2CN_2 have the same AFLOW prototype label. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Body-centered Tetragonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ca I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	P I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	P I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	U I
$\mathbf{B_5}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	U I

References

[1] 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.

[2] A. J. Locock and P. C. Burns, *The crystal structure of synthetic autunite, $Ca[(UO_2)(PO_4)]_2(H_2O)_{11}$*, Am. Mineral. **88**, 240–244 (2003), doi:10.2138/am-2003-0128.

Found in

[1] K. Herrmann, ed., *Strukturbericht Band VI 1938* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1941).