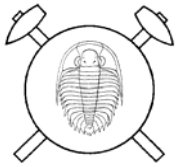
New naturally occurring phases of secondary origin from Jáchymov (Joachimsthal)

Nové sekundární minerální fáze z Jáchymova (Czech summary)



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This paper describes thirty inorganic compound – secondary mineral phases- found in the nature for the first time. All compounds come from the Jáchymov ore district. All up-to-now available physical and chemical data and references to appropriate literature are given. Crystal structure of phase [$(MoO_2)_2As_2O_5(H_2O)_2$] . H_2O was solved and refined, crystal structures of $Ca(H_2AsO_4)_2$ and Mg-villyaellenite were refined by the Rietveld method.

Key words: new natural phases, new data, secondary minerals, Jáchymov

Introduction

In the course of work on the project *Study of secondary minerals in the Jáchymov ore district* (1993 to 1997) [299] we have recognised and studied 30 inorganic phases, which were for the first time encountered as natural materials. This development prompted us to write this paper, dedicated exclusively to the new phases. Individual phases are characterised to variable degree, depending mainly on the type and quantity of material available.

Experimental methods

The experimental methods used in study of the new phases are the same as characterised in the paper presenting encyclopaedical review of Jáchymov minerals: *Secondary minerals of the Jáchymov ore district*. Additional methods used in study of the new phases include single crystal study and the Rietveld analysis of three new phases: [$(MoO_2)_2As_2O_5(H_2O)_2$] . H_2O (provisional designation ***MOASO***), $Ca(H_2AsO_4)_2$ (provisional designation ***CAS***) and "Mg-villyallenite".

Powder data (for Rietveld analysis) were collected using Philips X'Pert diffractometer equipped with copper sealed tube and graphite secondary monochromator. High voltage was set to 40 kV and tube current to 40 mA. Powder pattern was collected in range from 3 to 120 °2θ CuKα and step 0.01 °2θ CuKα with exposition of 10 sec. per step for ***CAS*** and in range from 3 to 130.005 °2θ CuKα with step 0.015 °2θ CuKα and exposition of 10 sec. per step in the case of ***MOASO***. To minimize complicated shape of background due to classic glass sample holders, the sample studied was placed on the surface of flat silicon wafer from alcoholic suspension.

Single peak profile fitting procedure using Pearson VII split asymmetric profile shape function implemented in the program ZDS ver. 6.01 [291] found angular positions and intensities of reflections in the powder pattern. Diffraction indices were assigned to yielded reflection positions based on theoretical powder pattern calculated from the crystal structure data with program FullProf (version 3.2 for PC-compatibles - [284]).

Lattice dimensions were refined from those data with program by Burnham [281] employing correction term $(\cos\theta.\cot\theta)/\lambda^2$ for sample displacement.

In the case of ***CAS*** and "Mg-villyallenite", program FullProf (version 3.2 for PC-compatibles - [284]) was used for the Rietveld refinement of crystal structure of this new mineral from experimentally measured powder X-ray diffraction data. Background was approximated via polynomial of the fifth order, corrections for sample displacement (cosine term) and preferred orientation (in March-Dollase form) were applied. Pseudo-Voigt profile shape function was utilized. Peak base was set to 5.5 FWHM.

For the single crystal X-ray measurement a needle-like fragment of ***MOASO*** was mounted on a glass fibre and measured using the four-circle diffractometer CAD4-MACHIII with MoKα radiation. The crystallographic data obtained are summarised in Tables. The crystal structure was solved by direct methods (SHELXS86 [287]) and refined by a full-matrix least-square procedure based on F^2 (SHELXL93, [288]). Scattering factors were those employed in the SHELX programs.

The qualitative, and in some cases quantitative, chemical composition of minerals was measured with the scanning electron microprobe CamScan 4 with an energy-dispersive analyser EDX system LINK eXL and a wave-dispersive analyser WDX system Microspec - 3PC.

For quantitative chemical analysis of mineral phases in the system Ca-Cu-UO_2-CO_3-H_2O the following conditions were used: the standards: azurite (Cu, C, O), calcite (Ca, C, O), uranium (U). Operating voltage and sample current 20 kV and 40 nA respectively. Specimen beam size was 15×10 μm.

For quantitative chemical analysis of ***MOASO*** the following conditions were used: the standards: arsenolite (As, O), molybdenum (Mo). Operating voltage and sample current 20 kV and 20 nA respectively. Specimen beam size was 5×5 μm.

Correction procedures ZAF, Phi(rho×Z), and Quadrilateral were used for calculation of all quantitative analyses.

TG, DTG curves were recorded simultaneously on the thermobalance TG 750 Stanton Redcroft. The operating conditions: sample weight about 1-3 mg, heating rate 10 °C.min^{-1}, dynamic air atmosphere 10 ml.min^{-1} and temperature range 20-1000 °C.

Infrared absorption spectra in the 400-4000 cm^{-1} range were recorded with and FTIR spectrometer Nicolet 740 using KBr pellets and/or diffusion reflection mode.

New naturally occurring phases

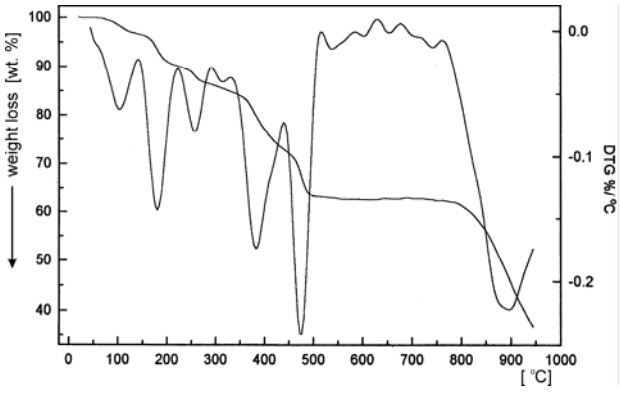
The phase: $[(Mo^{6+}O_2)_2As^{3+}{}_2O_5(H_2O)_2]\,.\,H_2O$ (MOASO)

It forms minute green to grey-green acicular crystals or continuous crusts, which rim strongly corroded veinlet. Laterally it gives way to grey-green scorodite in spherical and botryoidal aggregates. Sample number: J-230.

The phase was observed on fractures in proximity to strongly weathered arsenopyrite (löllingite)-pyrite vein approximately 5 cm thick, with the sulphides partly or completely altered to mixture of compact grey-black scorodite with a metallic lustre and arsenolite. Paragenesis: scorodite, parascorodite, arsenolite.

The specimens were collected in the Geschieber vein. The phase was formed in highly acid environment of concentrated sulphuric acid, in the presence of As_2O_3 in significant concentrations.

*Thermogravimetric (TG, DTG) curves of **MOASO** from Jáchymov*



*Crystal data and structure refinement for **MOASO***

Diffractometer	Enraf-Nonius CAD4-MACHIII
Empirical formula	$H_6\,As_2\,Mo_2\,O_{12}$
Formula weight	539.77
Temperature [K]	293(2)
Wavelength [Å]	0.71069
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	
a [Å]	7.0398(4)
b [Å]	12.0682(13)
c [Å]	12.210(2)
β [°]	101.265(9)
Volume [Å^3]	1017.4(2)
Z	4
Density (calculated) [g.cm^{-3}]	3.524
Absorption coefficient [mm^{-1}]	8.98
F(000)	1008
Crystal size [mm^3]	0.10 × 0.14 × 0.39
Theta range for data collection [°Θ]	2.40 to 24.99
Index ranges	
h	0; 8
k	0; 14
l	-14; 14
Reflections collected	1935
Independent reflections	1787 [R(int) = 0.0489]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1786 / 0 / 145
GOF	1.07
Final R indices [I>2σ(I)]	R1 = 0.0455, wR2 = 0.1143
R indices (all data)	R1 = 0.0580, wR2 = 0.1243
Δ/σ (max)	1.745
Δ(ρ) [e.A^{-3}]	-1.728

$R1 = \Sigma\,||F_o| - |F_c||\,/\,\Sigma|F_o|$

$wR2 = \{\Sigma[w(F_o^2-F_c^2)^2]\,/\,\Sigma[w(F_o^2)^2]\}^{0.5}$

$GOF = \{\Sigma[w(F_o^2-F_c^2)^2]/(N-P)\}^{0.5}$

*Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters [Å^2 × 10^3] for **MOASO**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.*

	x	**y**	**z**	**U_{eq}**
Mo(1)	6214(1)	2121(1)	2757(1)	12(1)
Mo(2)	1799(1)	2321(1)	905(1)	13(1)
As(3)	2066(1)	1418(1)	-1626(1)	13(1)
As(4)	6245(1)	3440(1)	5030(1)	13(1)
O(1)	-333(9)	2915(5)	1068(5)	24(2)
O(2)	4963(8)	1976(5)	1095(4)	14(1)
O(3)	1387(10)	951(5)	1006(5)	26(2)
O(4)	8084(9)	1267(5)	2671(5)	22(1)
O(5)	7186(9)	3414(5)	2745(5)	22(1)
O(6)	3147(8)	2659(5)	2485(4)	14(1)
O(7)	1681(9)	2432(5)	-668(5)	19(1)
O(8)	4275(8)	840(5)	-875(4)	14(1)
O(9)	6029(9)	2158(5)	4300(5)	18(1)
O(10)	4588(9)	470(5)	2832(5)	22(1)
O(11)	2886(11)	4090(6)	742(6)	34(2)
O(12W)	1477(9)	137(6)	3705(5)	25(2)

No mineral containing Mo was found in the assemblage. It is suggested that amorphous, finely dispersed Mo sulphides (jordisite) or oxides, soluble in the acid solutions, served as a source of Mo. The solutions carrying Mo^{6+} probably attained elevated concentrations which resulted in crystallisation of the new phase.

The quantitative chemical analysis: Mo 35.04, As 27.83, O 36.91 wt. % gives after recalculation based on 12 oxygen atoms the following empirical formula:

$$(MoO_2)_{1.93}(As_2O_5)_{0.95}(OH)_{0.07} \cdot 3.31\ H_2O$$

or a simplified formula:

$$(MoO_2)_2As_2O_5 \cdot 3\ H_2O$$

The crystal structure of ***MOASO*** was solved from single-crystal data (for details see Experimental methods at the beginning of this paper).

Polyhedral volumes and deformations expressed as bond angle variance, and quadratic elongation for two [MoO_6] octahedra in the crystal structure of ***MOASO***

	Mo1	**Mo2**
V_O [Å^3]	9.815	9.736
σ^2	129.738	121.352
Q.E.	1.0527	1.0505

Anisotropic displacement parameters [Å^2 × 10^3] for ***MOASO****. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}]$*

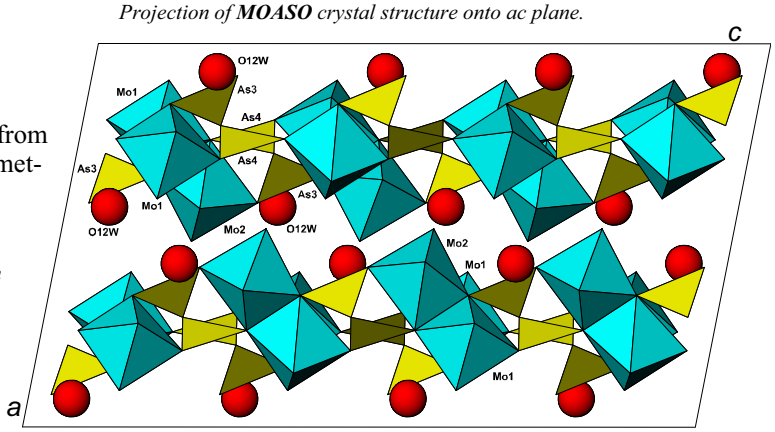
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mo(1)	9(1)	17(1)	7(1)	0(1)	-4(1)	2(1)
Mo(2)	10(1)	19(1)	7(1)	-1(1)	-4(1)	1(1)
As(3)	11(1)	18(1)	8(1)	-1(1)	-4(1)	-3(1)
As(4)	10(1)	20(1)	7(1)	0(1)	-3(1)	-3(1)
O(1)	18(3)	38(4)	10(3)	-2(3)	-8(3)	8(3)
O(2)	9(3)	25(3)	6(3)	2(2)	-1(2)	3(2)
O(3)	30(4)	19(3)	28(4)	0(3)	-1(3)	-1(3)
O(4)	18(3)	31(4)	14(3)	-4(3)	-5(2)	5(3)
O(5)	23(3)	20(3)	24(3)	3(3)	5(3)	-2(3)
O(6)	10(3)	26(3)	5(3)	-2(2)	-5(2)	4(2)
O(7)	16(3)	29(3)	8(3)	1(2)	-4(2)	4(3)
O(8)	15(3)	15(3)	11(3)	0(2)	-4(2)	3(2)
O(9)	15(3)	28(3)	6(3)	0(2)	-8(2)	1(3)
O(10)	20(3)	20(3)	22(3)	2(2)	-7(3)	-1(3)
O(11)	38(4)	25(4)	31(4)	0(3)	-10(3)	-11(3)
O(12W)	17(3)	26(4)	27(3)	-11(3)	-8(3)	-3(3)

Lattice par. [Å, °]	1	a = 7.0515(6)	b =12.0908(9)	c=12.2190(14)
			β=101.268(9)	
	2	a = 7.0398(4)	b=12.0682(13)	c=12.210(2)
			β=101.265(9)	
EDX, WDX		major elements: Mo, As	minor elements:	
Thermal anal. [°C, wt. %]		145 2.4, 247 4.23, 300 2.57, 360 1.54, 455 7.04, 624 10.82		
IR [cm^{-1}]		Drift: 433,475,522,543,587,678,751,799, 921,947,1023,1059,1122,1430,1620,2932, 2962,3137,3223,3424,3476,		
		KBr: 526,566,664,751,803,896,917,951, 1401,1623,1732,3117,3417,3478		
Density [g.cm^{-3}]	1	D_{cal} = 3.509(1), Z = 4		
	2	D_{cal} = 3.524		
References		252, 253, 281,284,285,286,287,288,291		

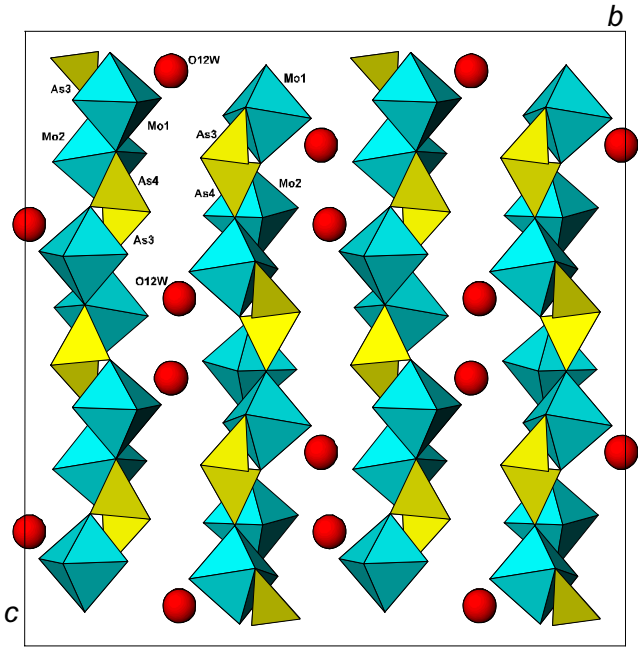
1 - single peak profile fitting from powder data
2 - single crystal data

Details on the structure are given in tables. Basic motif of the structure and projections of it onto ac and bc planes are presented in figures.

Projection of ***MOASO*** *crystal structure onto ac plane.*



Projection of ***MOASO*** *crystal structure onto bc plane.*



Aggregate of acicular crystals of the phase ***MOASO***. Magnification 150

The ***MOASO*** crystal structure consists of double-chains built up by two individual chains with a sequence ...O-As-O-Mo... interconnected by bridging oxygens and oxygen atoms belonging to a common apex of a bi-arsenite group. In intersticial spaces, there are water groups, probably comparable to channel or zeolitic water.

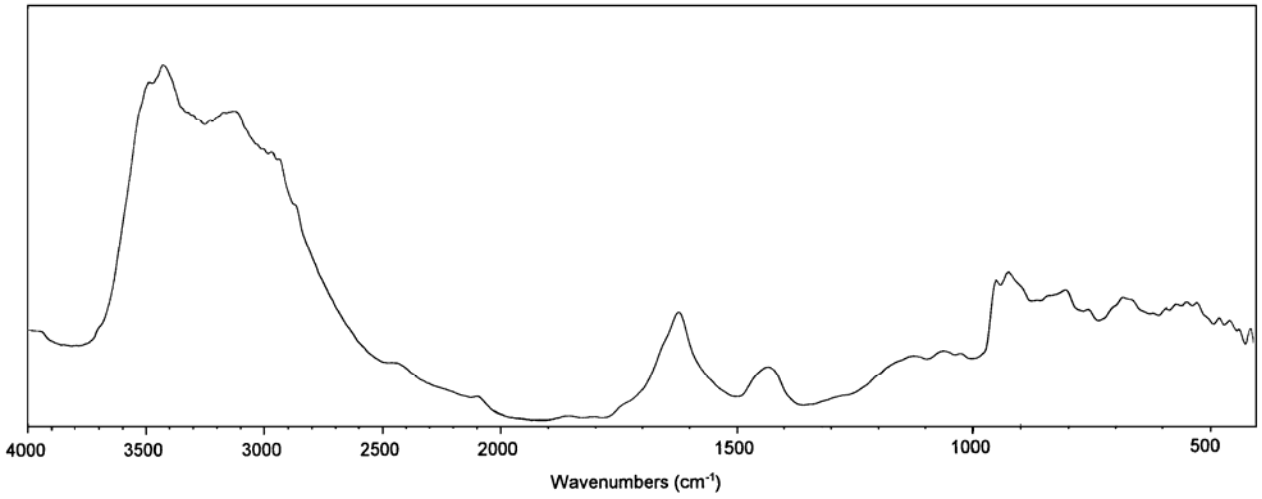
Two structurally non-equivalent [MoO_6] octahedra are slightly distorted as calculated from structure data by program VOLCAL [286] – see table. Polyhedron around Mo1 is of larger volume and also its quadratic elongation and bond-angle variance have higher values indicating more severe distortion than in the case of the octahedron around Mo2.

Bond lengths [Å] and angles [°] for ***MOASO***

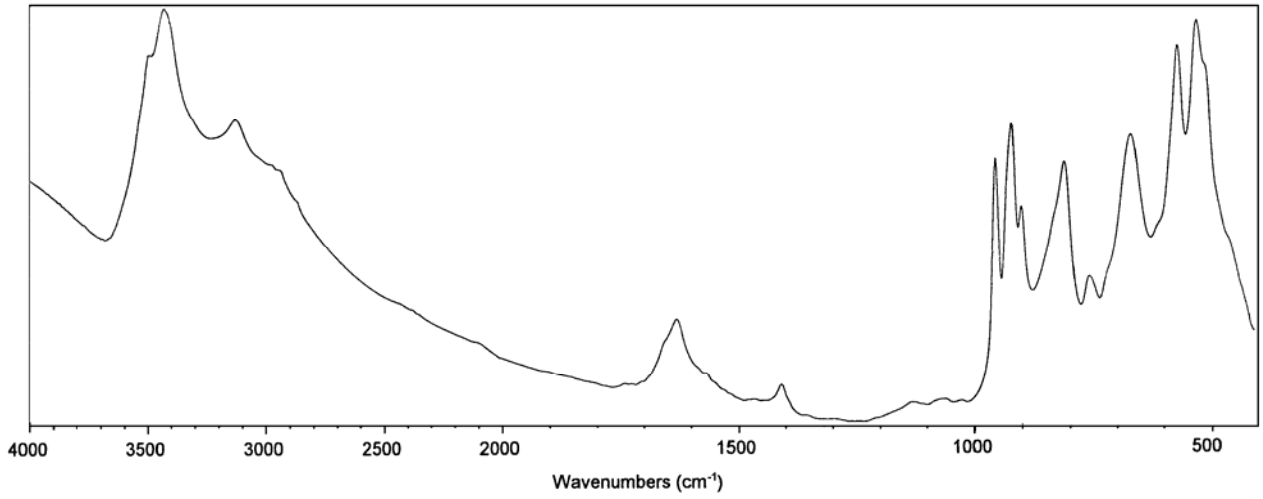
Mo(1)-O(4)	1.691(6)	As(4)-O(2)#2	1.793(6)	O(5)-Mo(1)-O(10)	173.2(3)	O(6)-Mo(2)-O(11)	78.0(2)
Mo(1)-O(5)	1.706(6)	As(4)-O(8)#2	1.817(5)	O(9)-Mo(1)-O(10)	81.4(2)	O(2)-Mo(2)-O(11)	80.8(2)
Mo(1)-O(9)	1.914(6)	O(2)-As(4)#1	1.793(6)	O(2)-Mo(1)-O(10)	81.1(2)	O(7)-As(3)-O(8)	99.4(3)
Mo(1)-O(2)	2.055(5)	O(6)-As(3)#2	1.823(6)	O(6)-Mo(1)-O(10)	77.4(2)	O(7)-As(3)-O(6)#1	96.2(3)
Mo(1)-O(6)	2.217(6)	O(8)-As(4)#1	1.817(5)	O(3)-Mo(2)-O(1)	103.6(3)	O(8)-As(3)-O(6)#1	97.0(3)
Mo(1)-O(10)	2.309(6)	O(4)-Mo(1)-O(5)	103.8(3)	O(3)-Mo(2)-O(7)	99.6(3)	O(9)-As(4)-O(2)#2	96.6(3)
Mo(2)-O(3)	1.687(6)	O(4)-Mo(1)-O(9)	106.2(3)	O(1)-Mo(2)-O(7)	102.8(3)	O(9)-As(4)-O(8)#2	97.6(2)
Mo(2)-O(1)	1.710(6)	O(5)-Mo(1)-O(9)	95.3(3)	O(3)-Mo(2)-O(6)	100.6(3)	O(2)#2-As(4)-O(8)#2	98.2(3)
Mo(2)-O(7)	1.911(6)	O(4)-Mo(1)-O(2)	94.3(3)	O(1)-Mo(2)-O(6)	93.7(3)	As(4)#1-O(2)-Mo(1)	124.1(3)
Mo(2)-O(6)	2.018(5)	O(5)-Mo(1)-O(2)	99.5(3)	O(7)-Mo(2)-O(6)	150.1(3)	As(4)#1-O(2)-Mo(2)	127.6(3)
Mo(2)-O(2)	2.233(5)	O(9)-Mo(1)-O(2)	151.0(2)	O(3)-Mo(2)-O(2)	89.5(3)	Mo(1)-O(2)-Mo(2)	108.3(2)
Mo(2)-O(11)	2.289(7)	O(4)-Mo(1)-O(6)	156.4(3)	O(1)-Mo(2)-O(2)	161.2(3)	As(3)#2-O(6)-Mo(2)	121.3(3)
As(3)-O(7)	1.750(6)	O(5)-Mo(1)-O(6)	96.4(3)	O(7)-Mo(2)-O(2)	87.9(2)	As(3)#2-O(6)-Mo(1)	126.7(3)
As(3)-O(8)	1.786(5)	O(9)-Mo(1)-O(6)	83.6(2)	O(6)-Mo(2)-O(2)	70.4(2)	Mo(2)-O(6)-Mo(1)	110.3(3)
As(3)-O(6)#1	1.822(6)	O(2)-Mo(1)-O(6)	70.1(2)	O(3)-Mo(2)-O(11)	170.1(3)	As(3)-O(7)-Mo(2)	129.9(4)
As(4)-O(9)	1.778(6)	O(4)-Mo(1)-O(10)	82.8(3)	O(1)-Mo(2)-O(11)	86.3(3)	As(3)-O(8)-As(4)#1	127.6(3)
				O(7)-Mo(2)-O(11)	78.3(3)	As(4)-O(9)-Mo(1)	119.9(3)

Symmetry transformations used to generate equivalent atoms: x,-y+1/2,z-1/2 ; x,-y+1/2,z+1/2

Infrared absorption spectrum (drift) of ***MOASO*** *from Jáchymov*



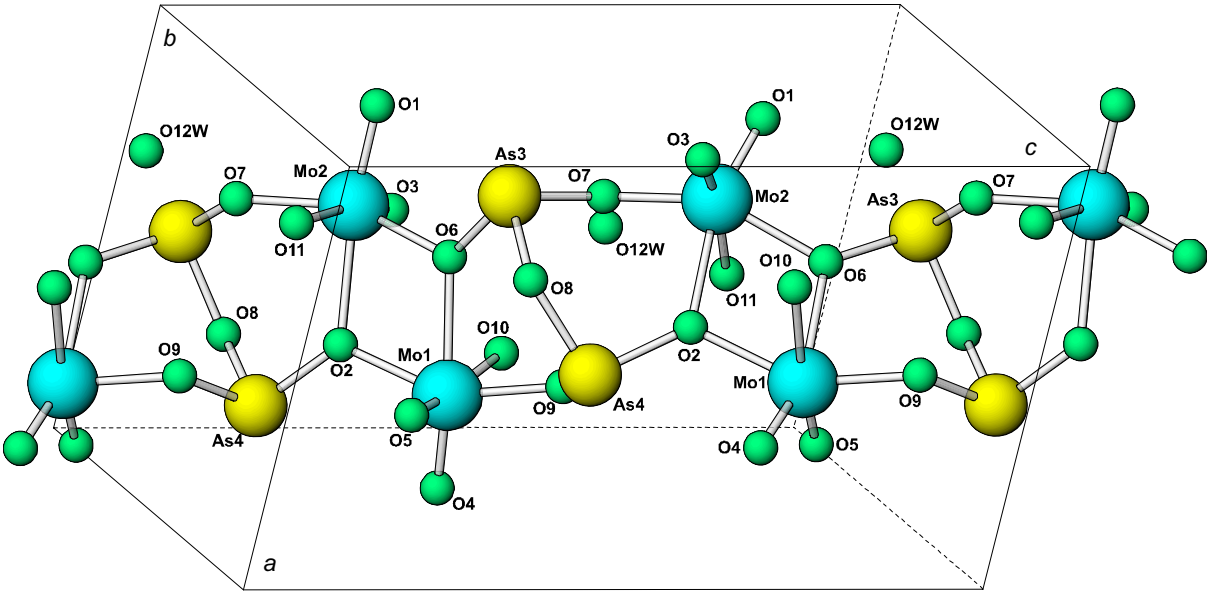
Infrared absorption spectrum (KBr tablet) of ***MOASO*** *from Jáchymov*



X-ray powder diffraction pattern of $[(MoO_2)_2As_2O_5(H_2O)_2]$. H_2O from Jáchymov.

I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*	I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*	I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*
3	8.524	8.511	0	1	1	5	1.9866	1.9872	0	6	1	1	1.3633	1.3630	1	4	-8
26	6.915	6.916	1	0	0	<1	1.9343	1.9347	1	6	0	4	1.3485	1.3483	5	2	0
100	6.046	6.045	0	2	0	3	1.9264	1.9266	1	6	-1	1	1.3304	1.3324	2	4	-8
4	5.776	5.774	1	1	-1			1.9246	3	3	-3	<1	1.3279	1.3304	5	3	-2
2	5.040	5.042	1	0	-2	7	1.9201	1.9208	2	5	1			1.3294	1	3	8
		5.036	1	1	1	1	1.8967	1.8975	2	0	-6			1.3290	1	5	7
7	4.551	4.551	1	2	0			1.8964	0	2	6			1.3278	5	2	-4
8	4.458	4.449	1	2	-1	0	1.8778	1.8780	0	4	5			1.3269	2	7	4
2	4.081	4.084	1	2	1			1.8763	2	4	3	1	1.3188	1.3183	1	6	-7
6	3.922	3.921	1	1	2	3	1.8710	1.8712	1	6	-2			1.3188	1	9	0
4	3.874	3.872	1	2	-2	1	1.8551	1.8555	3	4	-1	1	1.3057	1.3047	0	6	7
10	3.819	3.820	0	3	1	3	1.8342	1.8343	3	4	-2			1.3056	1	9	1
16	3.457	3.458	2	0	0	<1	1.7365	1.7368	4	1	-2			1.3053	4	6	-3
4	3.434	3.436	1	3	-1	3	1.7289	1.7289	4	0	0	1	1.2639	1.2639	3	8	0
59	3.324	3.333	0	2	3	5	1.7115	1.7115	4	1	0			1.2632	3	7	-5
		3.325	2	1	0			1.7094	2	4	4	1	1.2549	1.2547	2	9	-1
2	3.260	3.259	1	3	1	<1	1.7048	1.7050	1	6	3			1.2538	4	1	-8
1	3.214	3.214	1	2	-3	1	1.6857	1.6855	3	5	-1	1	1.24387	1.24380	4	6	2
<1	3.059	3.059	2	1	1			1.6844	3	4	-4	1	1.23672	1.23643	2	9	1
1	3.021	3.023	0	4	0	4	1.6757	1.6758	1	7	0			1.23486	3	2	7
7	3.000	3.002	2	2	0			1.6756	3	0	4	<1	1.20874	1.20874	2	9	2
		2.996	0	0	4	3	1.6696	1.6695	3	5	-2	<1	1.20307	1.20308	4	3	-8
2	2.930	2.931	0	4	1	3	1.6621	1.6647	3	1	-6	2	1.20027	1.20166	2	1	-10
3	2.909	2.908	0	1	4			1.6597	3	1	4			1.20218	0	6	8
5	2.887	2.890	1	3	2			1.6623	4	2	0	1	1.18912	1.18912	1	10	-1
		2.887	2	2	-2	1	1.6433	1.6428	4	0	-4	2	1.16663	1.16635	3	9	-1
		2.883	1	1	-4	1	1.6294	1.6295	2	6	2			1.16618	5	1	4
1	2.828	2.830	2	1	-3	2	1.6060	1.6059	4	2	1	2	1.15313	1.15287	5	6	-1
		2.827	1	2	3	1	1.5887	1.5889	4	3	0			1.15365	6	2	-2
9	2.801	2.802	2	2	1	1	1.5858	1.5853	4	2	-4	2	1.14840	1.14867	6	2	-3
2	2.768	2.770	2	0	2			1.5856	2	1	6			1.14872	6	1	-4
3	2.745	2.746	1	4	-1	2	1.5763	1.5768	4	3	-3	1	1.14129	1.14131	2	10	0
15	2.624	2.624	2	3	0			1.5757	0	3	7			1.14189	1	8	-7
12	2.593	2.593	1	4	-2			1.5757	3	4	3	1	1.13214	1.13299	0	8	7
1	2.573	2.572	1	0	4	<1	1.5719	1.5721	1	7	-3			1.13341	4	8	-3
5	2.515	2.518	2	2	2	3	1.5499	1.5498	2	7	-1	1	1.12189	1.12360	6	3	-3
		2.516	1	1	4			1.5473	1	6	-5	1	1.11945	1.11977	1	10	-4
2	2.4871	2.4876	2	3	1	1	1.5393	1.5415	2	6	3			1.12006	3	9	-4
2	2.3658	2.3666	1	2	4			1.5409	4	1	-5	1	1.02939	1.02928	5	8	-1
		2.3644	1	4	-3	1	1.5298	1.5270	1	0	-8	<1	1.02136	1.02143	4	2	8
<1	2.3261	2.3269	2	2	-4			1.5295	4	2	2			1.02165	2	11	2
2	2.3047	2.3052	3	0	0	4	1.5162	1.5172	3	6	0			1.02056	3	7	-9
8	2.2824	2.2827	2	3	2			1.5150	1	1	-8	<1	1.01970	1.01980	3	8	6
		2.2826	1	5	0			1.5158	2	7	1			1.01967	2	10	-6
19	2.2642	2.2644	3	1	0	3	1.4998	1.4995	0	8	1			1.01925	1	7	9
2	2.2425	2.2429	1	2	-5	1	1.4808	1.4805	1	2	-8	<1	0.99776	0.99733	6	4	-7
		2.2424	0	5	2	1	1.4764	1.4781	3	2	-7	2	0.99595	0.99607	4	9	3
1	2.1957	2.1970	1	4	3			1.4765	1	8	0			0.99593	6	5	2
2	2.1850	2.1907	3	2	-1	2	1.4728	1.4734	4	1	3			0.99592	1	12	-1
		2.1849	2	4	1			1.4729	1	8	-1			0.99567	3	11	-1
1	2.1559	2.1561	3	2	-2			1.4703	3	5	-5			0.99566	4	10	-2
		2.1554	3	1	-3	2	1.4587	1.4589	4	4	1	<1	0.98820	0.98794	7	0	0
<1	2.1366	2.1374	2	3	-4	2	1.4011	1.3987	1	1	8	3	0.98470	0.98474	4	3	-11
3	2.0890	2.0887	1	5	2			1.4009	4	4	2			0.98527	0	2	12
1	2.0412	2.0421	2	4	2	2	1.3920	1.3930	4	3	3			0.98459	0	7	10
1	2.0298	2.0273	1	0	-6			1.3919	3	7	-1			0.98466	7	1	0
7	2.0011	2.0028	3	3	-2	6	1.3835	1.3831	5	0	0						
		2.0010	3	3	0												

*Basic structure motif found in the **MOASO** crystal structure*



X-ray powder diffraction pattern of Ca-(VO)-AsO_4 from Jáchymov.

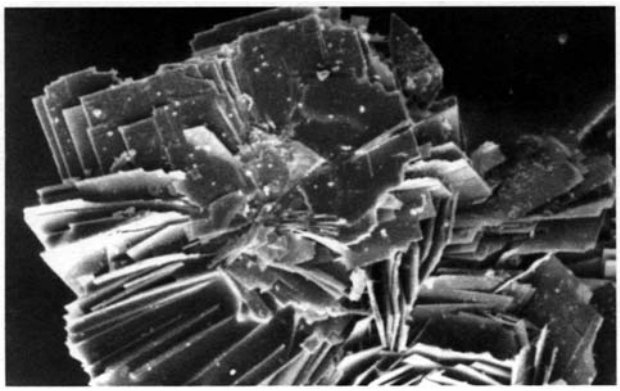
I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
4.4	10.390	3.0	4.973	0.4	3.802	1.4	2.949	8.8	2.1432
2.5	9.945	0.4	4.730	2.1	3.586	0.3	2.830	0.9	1.9909
2.2	9.446	0.5	4.538	0.6	3.504	0.5	2.801	0.7	1.9295
4.4	9.047	0.8	4.466	5.1	3.344	0.8	2.657	0.6	1.8181
2.9	7.605	1.1	4.258	0.5	3.317	1.0	2.518	0.5	1.8043
1.3	7.078	0.5	4.177	51.7	3.214	0.6	2.4534	0.7	1.6201
100.0	6.433	1.8	4.071	0.9	3.042	0.5	2.2831	0.7	1.6058
2.4	5.204	0.8	3.846	0.5	3.005	0.6	2.2581		

The phase: Ca-(VO)-AsO_4

The phase Ca-(VO)-AsO_4 occurs predominantly as inconspicuous aggregates consisting of very thin tetragonal crystal in rose-like clusters.

Imperfectly developed individual very thin crystals based on wall rock matrix are less common. It does not fluoresce in ultra-violet light. Specimen number: J-270.

EDX, WDX		major elements: Ca, As, V	minor elements:
References		22	



Aggregate of thin tabular crystals of the phase Ca-(VO)-AsO_4. Magnification 90

The phase Ca-(VO)-AsO_4 was always found aside from other loosely associated minerals, in particular vanadium minerals. This apparently indicates its increased solubility. The solutions transporting ions of this phase were probably relatively concentrated at margins of fractures. A local change in pH possibly also influenced the transport of ions.

The specimens of the phase were collected in the Geister vein.

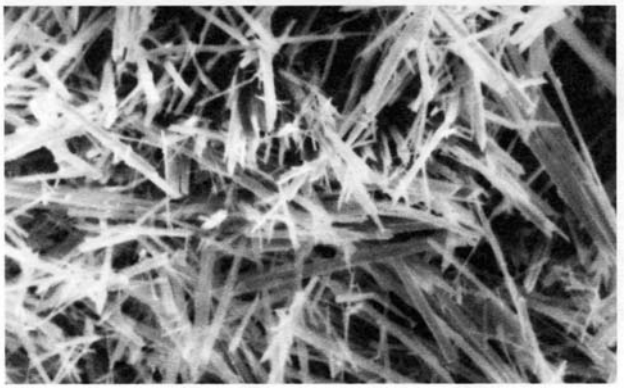
The phase: Ca-Mg-AsO_4-H_2O

It forms soft aggregates of randomly oriented minute acicular crystals, which can be easily overlooked as they are similar to picropharmacolite, mineral usually associated and mixed with this phase. The single difference in appearance in a specimen is that the crystals of the phase Ca-Mg-AsO_4-H_2O (sample: J-252) are distinctly shorter. Additional occurrences in the Jáchymov district or at some other localities can be expected. In fact, the same phase was identified at an earlier date on a specimen from Příbram as a fan-shaped aggregate, in this case of longer and wider crystals. The phase J-252 forms, similar to pharmacolite, at early stages of weathering of arsenide ores.

EDX, WDX		major elements: Ca, Mg, As	minor elements:
References		107, 130, 131, 132, 265	

X-ray powder diffraction pattern of Ca-Mg-AsO_4-H_2O from Jáchymov.

I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
100	11.95	5	5.374	46	3.551	32	2.955	10	2.206
12	10.05	14	4.966	11	3.398	26	2.804	4	2.104
33	7.92	13	4.330	7	3.330	16	2.708	7	1.991
14	6.77	8	3.988	34	3.246	8	2.599	2	1.938
7	5.96	15	3.956	8	3.144	8	2.523	7	1.897
4	5.596	23	3.794	16	3.067	3	2.432	3	1.786
								6	1.747



Acicular crystals of the phase Ca-Mg-AsO_4-H_2O. Magnification 500

Dehydration of the phase, proceding already at room temperature, results in picropharmacolite. The probably irreversible process may take in a dry and relatively warm environment some months to years. However, the phase J-252 was identified also in a specimen kept in collection for over 100 years.

The phase: $Ca(H_2AsO_4)_2$ - CAS [calcium bis(dihydrogen arsenate)]

Turning-on sequence of the parameters refined in the Rietveld crystal structure refinement of $Ca(H_2AsO_4)_2$.

Scale factor	1
Sample displacement	2
Backgound polynomial coefficients	3, 4, 5, 15, 56, 60
Ca *x, y, z,* B_{iso}	16, 19, 22, 49
As1 *x, y, z,* B_{iso}	17, 20, 23, 50
As2 *x, y, z,* B_{iso}	18, 21, 24, 51
O1 *x, y, z,* B_{iso}	25, 33, 41, 53
OH2 *x, y, z,* B_{iso}	26, 34, 42, 52
OH3 *x, y, z,* B_{iso}	27, 35, 43, 52
O4 *x, y, z,* B_{iso}	28, 36, 44, 53
OH5 *x, y, z,* B_{iso}	29, 37, 45, 52
O6 *x, y, z,* B_{iso}	30, 38, 46, 53
OH7 *x, y, z,* B_{iso}	31, 39, 47, 52
OH8 *x, y, z,* B_{iso}	32, 40, 48, 52
pseudo-Voigt PSF parameters	54, 57
U, V, W	14, 13, 6
Lattice parameters	7, 8, 9, 10, 11, 12
Preferred orientation parameters	58
Asymmetry coefficients	55, 59

The phase $Ca(H_2AsO_4)_2$ occurs typically as clear transparent coating composed of indistinct radiating aggregates with a glassy lustre. The needles are oriented parallel to the surface of the coating. The inconspicuous coatings are relatively strong, up to 2 mm thick and produce a white streak. The material also forms hollow botryoidal crusts with a mat or lustrous surface.

The phase tends to occur isolated from other arsenates common in Jáchymov. However, the white crusts contain as yet unidentified phase with probable composition Ca-Mg-AsO_4-H_2O. This would correspond to chemical composition and the mode of formation.

The phase $Ca(H_2AsO_4)_2$ crystallised from relatively concentrated, strongly acidic solutions with a relatively strong circulation, which carried arsenic acid produced by decomposition of rich accumulations of native arsenic or arsenides.

Conditions and results of the Rietveld crystal structure refinement of $Ca(H_2AsO_4)_2$

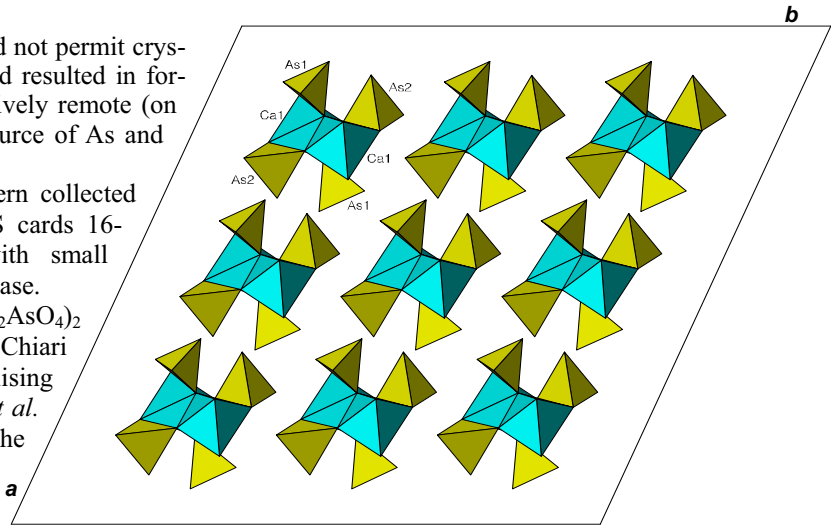
Formula	$Ca(H_2AsO_4)_2$
Diffractometer	Philips X'Pert System MPD
Wavelengths, λ (Å)	1.5405 + 1.5443
2θ range (°2θ)	3-120
Step width (°2θ)	0.01
Counting time (sec.)	10
No. of observations	11701
No. of reflections	1952
No. of structural variables	39
No. of profile variables	14
No. of global variables	7
Excluded regions (°2θ)	3-10.7, 17.62-18.02, 20.7-21, 25.44-25.6, 25.95-26.95
Space group	$P\bar{1}$
Lattice parameters	
a (Å)	8.5483(3)
b (Å)	7.6975(3)
c (Å)	5.7196(2)
α (°)	92.598(2)
β (°)	109.871(2)
γ (°)	109.912(2)
Z	2
D_x (g.cm^{-3})	3.2676(2)
FWHM at 42.56° (°2θ)	0.1086
Average FWHM (°2θ)	0.1873
U, V, W	0.056(6), -0.044(5), 0.020(1)
R_{wp} (%)	8.40
R_p (%)	6.55
R_{exp} (%)	2.62
R_B (%)	14.60
R_F (%)	10.30
χ^2	10.30
Convergence criterion, ε	0.10

The increased acidity of solution did not permit crystallisation of the common arsenates and resulted in formation of $Ca(H_2AsO_4)_2$ in places relatively remote (on the order of metres) of the primary source of As and Ca.

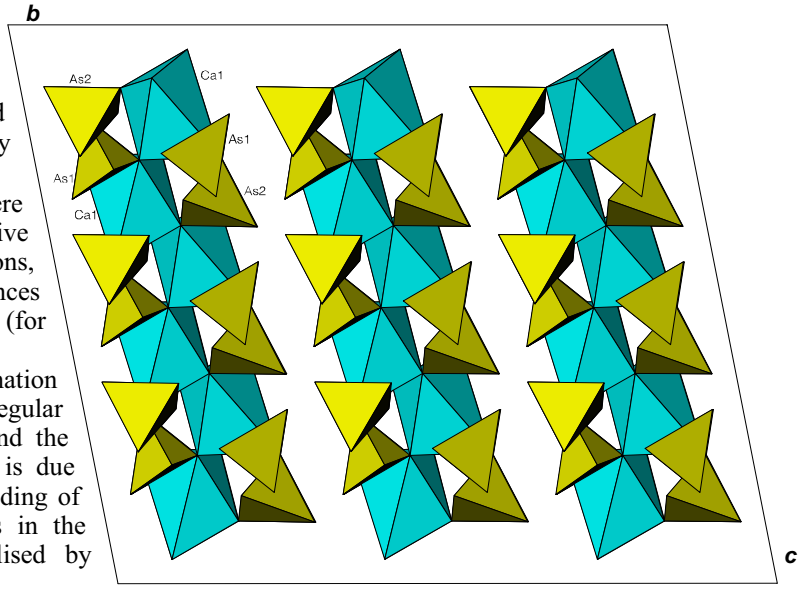
The powder X-ray diffraction pattern collected has revealed the identity with JCPDS cards 16-0691 and 44-0279, respectively, with small admixture of an unknown crystalline phase.

Crystal structure of synthetic $Ca(H_2AsO_4)_2$ was originally solved and refined by Chiari and Ferraris [282] without localising hydrogen atoms and later on Ferraris *et al.* [283] localised hydrogen atoms within the crystal structure using neutron single crystal data.

The former structure was eventually used as a starting model for the Rietveld crystal structure refinement of naturally occurring calcium bis(dihydrogen arsenate) from Jáchymov.



Projection of the $Ca(H_2AsO_4)_2$ crystal structure onto ab plane.



Projection of the $Ca(H_2AsO_4)_2$ crystal structure onto bc plane.

Crystal structure of $Ca(H_2AsO_4)_2$ consists chains built up by zig-zag arranged pairs of $[CaO_6]$ octahedra sharing one corner and slightly tilted which are mutually interconnected by $[AsO_4]$ tetrahedra.

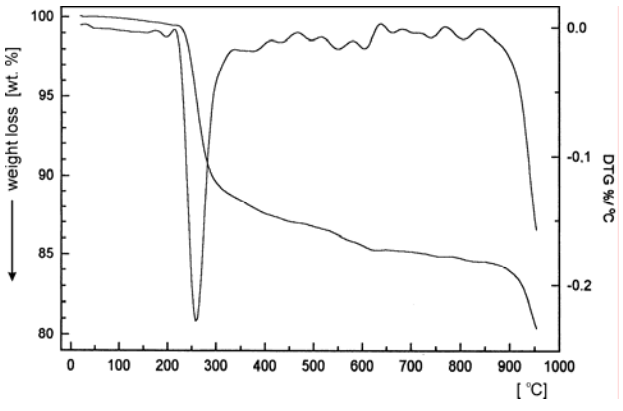
Two different tetrahedra were characterised in terms of their respective polyhedral volumes, quadratic elongations, bond angle and bond distance variances using program VOLCAL [286] (for definition of these parameters see [285]).

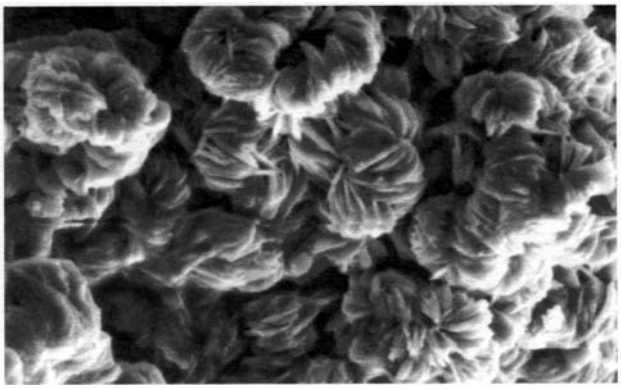
These parameters show that coordination tetrahedron around As2 atom is more regular and significantly larger than that around the other arsenic atom. This phenomenon is due most probably to different types of bonding of these coordination polyhedra which is in the case of tetrahedron around As2 realised by hydrogen bridges.

Lattice par. [Å, °]	1	a= 8.5483(3)	b= 7.6975(3)	c= 5.7196(2)
		α=92.598(2)	β=109.871(2)	γ=109.912(2)
	2	a= 8.5485(9)	b= 7.6973(7)	c= 5.7198(5)
		α=92.595(7)	β=109.876(6)	γ=109.920(6)
EDX, WDX		major elements: Ca, As	minor elements: (Mg)	
Therm. analysis [°C, wt. %]		215-335 10.5 (loss of H_2O)		
IR [cm^{-1}]		Drift:413,431,530,590,629,712,740,776,814, 870,912,992,1138,1234,1402,1626,2387,2499 ,3006,3094,3365		
		KBr:536,711,745,807,882,913,999,1077,1133 1234,1385,1487,1635,2386,2930,2965,3371		
Density [$g.cm^{-3}$]	1	D_{cal} = 3.2676(2), Z = 2		
	2	D_{cal} = 3.2678(8)		
References		275,281,282,283,284,285,286,291		

1) data from the Rietveld refinement
2) data from single peak profile fitting

Thermogravimetric (TG,DTG) curves of $Ca(H_2AsO_4)_2$ from Jáchymov





Rosette-shaped aggregates of tabular crystals of the phase ***CAS***. Magnification 800

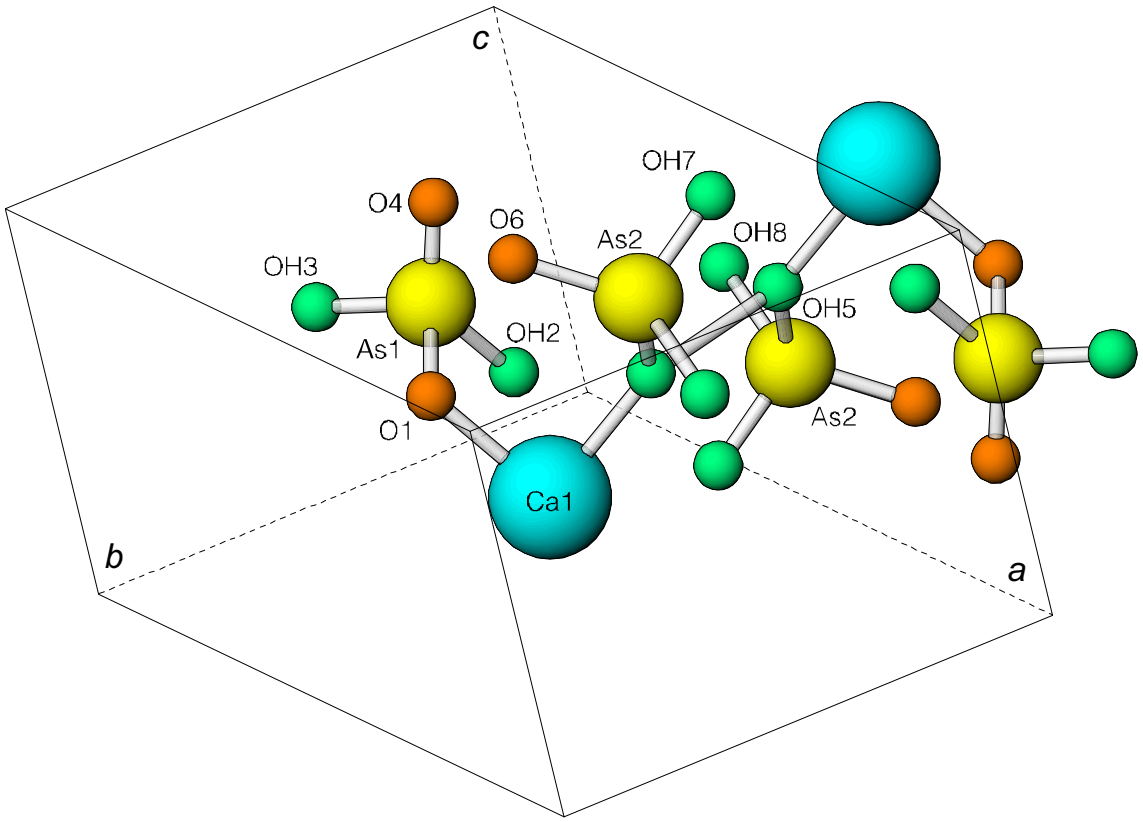
Polyhedral volumes and deformations expressed as bond angle variance, bond distance variance, and quadratic elongation for two [AsO_4] tetrahedra in the crystal structure of $Ca(H_2AsO_4)_2$

	As1	**As2**
V_T [Å^3]	2.681	3.389
σ^2	177.34	51.45
Δ	10.07	8.26
Q.E.	1.0516	1.0300

Fractional coordinates and isotropic temperature factors [Å^2] for naturally occurring $Ca(H_2AsO_4)_2$ from the Rietveld crystal structure refinement.

	x	σ_x	y	σ_y	z	σ_z	B_{iso}	σ_B		x	σ_x	y	σ_y	z	σ_z	B_{iso}	σ_B
Ca1	0.0777	0.0007	0.1784	0.0007	0.3096	0.0011	0.3	0.1	OH3	0.5418	0.0018	0.1837	0.0019	0.0876	0.0025	1.2	0.2
As1	0.3359	0.0005	0.2410	0.0005	-0.0135	0.0007	1.4	0.1	O4	0.3098	0.0020	0.2717	0.0021	-0.2730	0.0031	2.6	0.3
As2	0.1827	0.0004	0.7661	0.0004	0.3289	0.0006	1.1	0.1	OH5	0.0434	0.0019	0.6709	0.0019	0.0022	0.0029	1.2	0.2
O1	0.1478	0.0019	0.0557	0.0022	0.0233	0.0030	2.6	0.3	O6	0.1050	0.0021	0.9227	0.0021	0.4669	0.0032	2.6	0.3
OH2	0.3924	0.0020	0.4081	0.0020	0.2877	0.0026	1.2	0.2	OH7	0.1546	0.0018	0.5645	0.0020	0.4731	0.0027	1.2	0.2
OH8	0.4447	0.0019	0.8830	0.0020	0.2943	0.0028	1.2	0.2	OH8	0.4447	0.0019	0.8830	0.0020	0.2943	0.0028	1.2	0.2

Basic structure motif found in the $Ca(H_2AsO_4)_2$ crystal structure



X-ray powder diffraction pattern of $Ca(H_2AsO_4)_2$ from Jáchymov.

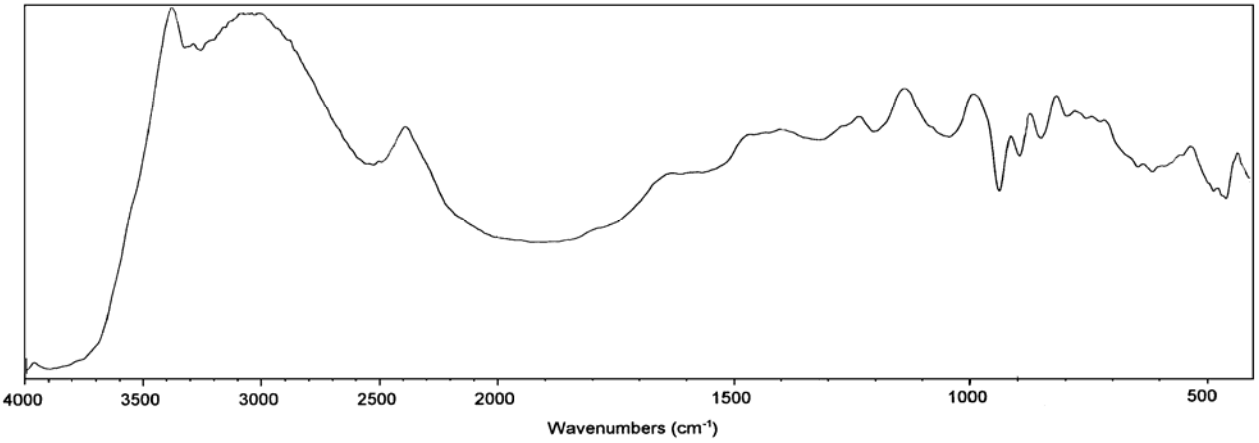
I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*	I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*	I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*
12	7.460	7.439	1	0	0	9	1.5996	1.6003	0	4	1	5	1.18252	1.18286	2	-5	3
29	7.141	7.116	0	1	0			1.6001	1	-2	-3			1.18305	6	-4	-3
29	6.530	6.524	1	-1	0	2	1.5819	1.5814	5	-1	0			1.18208	7	-1	-1
2	5.380	5.377	1	0	-1	<1	1.5793	1.5776	4	0	1	<1	1.18100	1.18035	1	-6	-1
6	5.295	5.289	0	0	1	7	1.5760	1.5765	5	0	-2	11	1.16970	1.16979	5	-6	-1
12	4.675	4.672	0	1	-1			1.5761	4	-2	-3	8	1.16738	1.16793	5	-6	0
42	4.490	4.486	1	-1	-1	13	1.5575	1.5583	3	-4	-2			1.16772	6	-1	-4
40	4.119	4.118	1	1	-1	6	1.5500	1.5501	2	-4	2			1.16755	0	5	2
72	3.974	3.972	2	-1	0	13	1.5456	1.5463	3	3	-1	3	1.16481	1.16498	5	3	-2
24	3.920	3.917	0	1	1			1.5460	1	4	-2	8	1.16289	1.16311	5	-4	2
4	3.823	3.823	1	-2	0	2	1.5424	1.5412	3	0	2			1.16264	1	1	4
29	3.812	3.813	1	-1	1	41	1.5379	1.5379	2	-5	0			1.16230	7	-4	-1
29	3.792	3.792	-2	0	1			1.5368	5	-3	-2	4	1.15633	1.15625	4	-2	3
37	3.771	3.770	2	-1	-1	6	1.5281	1.5286	4	1	-3	2	1.15344	1.15350	7	-4	-2
29	3.722	3.720	2	0	0	2	1.5091	1.5097	3	3	-2			1.15338	7	-1	-3
60	3.700	3.700	1	0	1			1.5089	2	3	1	2	1.15133	1.15140	4	4	-1
100	3.558	3.558	0	2	0	8	1.5067	1.5069	3	2	1			1.15168	0	4	3
85	3.262	3.262	2	-2	0	3	1.4819	1.4823	2	3	-3	1	1.14816	1.14855	3	-6	2
5	3.237	3.238	0	2	-1	26	1.4760	1.4783	2	-3	-3	5	1.14623	1.14677	4	-3	3
82	3.101	3.100	1	-2	1			1.4764	1	-4	-2			1.14647	6	0	-4
62	3.041	3.039	2	1	-1			1.4763	0	2	3	2	1.14459	1.14400	1	-3	-4
25	3.006	3.006	2	-2	-1			1.4750	5	-4	-1			1.14416	7	-2	0
30	2.926	2.926	1	1	1	4	1.4604	1.4598	3	3	0	1	1.14123	1.14124	3	0	-5
44	2.879	2.879	2	1	0	20	1.4521	1.4541	5	1	-1	5	1.13586	1.13637	2	-5	-3
38	2.856	2.856	1	0	-2			1.4540	2	-2	3			1.13587	4	-1	3
		2.853	1	2	-1			1.4539	4	-3	-3	2	1.13030	1.13035	3	4	1
2	2.820	2.820	1	2	0			1.4520	5	1	-2	3	1.12831	1.12812	3	3	2
16	2.804	2.805	3	-1	-1	6	1.4454	1.4459	1	3	2	4	1.12031	1.12146	-4	4	4
6	2.730	2.731	0	2	1	9	1.4319	1.4319	3	-4	2			1.12015	6	-3	-4
22	2.699	2.699	1	1	-2	<1	1.4269	1.4280	2	0	-4	4	1.11735	1.11716	1	1	-5
52	2.666	2.666	3	0	-1	5	1.4226	1.4231	0	5	0	7	1.11620	1.11643	6	2	-1
6	2.641	2.641	0	1	-2	4	1.4190	1.4193	4	-5	0			1.11583	-7	0	3
8	2.612	2.613	2	0	1			1.4180	6	-2	-1	1	1.10962	1.10951	4	-4	3
21	2.591	2.592	2	-1	-2	<1	1.4131	1.4142	2	1	-4	2	1.10057	1.10082	5	2	1
		2.592	2	-2	1	12	1.4096	1.4102	2	4	0			1.10002	1	2	-5
19	2.556	2.556	3	-2	-1			1.4098	3	1	2	1	1.09918	1.09914	6	1	-4
5	2.535	2.534	3	-2	0			1.4089	-3	0	4	6	1.09138	1.09139	2	-7	0
1	2.4816	2.4798	3	0	0			1.4070	1	-5	-1	6	1.08717	1.08809	2	-4	4
12	2.4681	2.4686	2	-3	0	2	1.4006	1.4011	2	0	3			1.08725	6	-6	0
10	2.3715	2.3719	0	3	0			1.4011	5	-4	-2	7	1.08109	1.08128	3	-7	1
15	2.3651	2.3650	1	-3	1	7	1.3943	1.3947	2	-3	3			1.08092	4	-7	0
1	2.3417	2.3433	0	1	2			1.3944	6	-1	-1	6	1.07734	1.07817	2	3	3
19	2.3277	2.3284	0	3	-1	4	1.3862	1.3865	2	-1	-4			1.07763	5	-1	-5
16	2.3155	2.3165	3	-1	-2	15	1.3839	1.3847	0	4	-3			1.07725	1	5	2
		2.3158	2	2	-1			1.3840	5	-1	1	5	1.06923	1.06783	7	-1	-4
18	2.2908	2.2916	2	-3	-1	4	1.3797	1.3803	1	-5	2	2	1.06522	1.06538	3	-2	4
28	2.2843	2.2852	1	2	-2	1	1.3724	1.3727	3	3	-3	5	1.06278	1.06372	1	5	-4
8	2.2726	2.2722	3	1	-1	10	1.3460	1.3465	1	5	-1			1.06311	6	-3	2
4	2.2439	2.2450	1	-3	-1	1	1.3444	1.3444	4	0	-4	<1	1.06278	1.06228	1	3	-5
8	2.2364	2.2387	1	0	2	2	1.3403	1.3396	1	-1	-4	2	1.05951	1.05936	8	-3	-1
		2.2357	1	2	1	4	1.3389	1.3391	6	-2	0	3	1.05210	1.05191	7	-3	1
6	2.2104	2.2110	2	1	1	<1	1.3295	1.3292	3	-5	-2	4	1.04933	1.04974	5	1	-5
6	2.1891	2.1860	2	-3	1	9	1.3234	1.3240	6	-3	0	3	1.04461	1.04428	6	1	1
48	2.1731	2.1735	1	-2	-2			1.3236	6	0	-1	6	1.03792	1.03846	5	4	-2
13	2.1218	2.1223	3	-2	-2			1.3227	3	-4	-3	3	1.03594	1.03613	1	-7	2
18	2.1062	2.1024	1	3	-1			1.3222	0	0	4	5	1.03468	1.03492	2	5	-4
9	2.0860	2.0861	3	-2	1	6	1.3181	1.3183	5	-5	-1			1.03463	6	2	-4
8	2.0763	2.0774	4	-2	-1	2	1.3099	1.3104	4	-5	-2	1	1.03317	1.03340	3	-6	3
1	2.0586	2.0590	2	2	-2			1.3096	4	-4	-3	3	1.03204	1.03269	8	-3	-3
2	2.0296	2.0305	0	3	1	6	1.3060	1.3065	5	2	-2	3	1.02720	1.02720	4	1	3
5	2.0089	2.0084	4	0	-1			1.3064	4	0	2	3	1.02394	1.02429	8	-1	-1
46	1.9930	1.9938	4	-1	0	<1	1.3060	1.3054	2	1	3	3	1.02310	1.02328	2	-5	4
12	1.9846	1.9860	4	-2	0	1	1.3018	1.3024	2	-2	-4			1.02322	2	6	0
27	1.9758	1.9761	3	0	1	8	1.3003	1.3005	3	2	-4	3	1.01987	1.01914	1	-2	-5
4	1.9610	1.9610	4	-1	-2			1.3005	6	-2	-3	4	1.01571	1.01541	1	-7	-1
10	1.9458	1.9464	2	-1	2			1.3007	1	5	-2	3	1.00448	1.00423	6	-5	2
15	1.9110	1.9114	2	-4	0	1	1.2982	1.2986	2	4	-3	3	1.00032	1.00006	7	-5	1
9	1.9015	1.9027	1	-3	2	5	1.2961	1.2968	2	-4	3	4	0.99724	0.99688	8	-2	0

To be continued

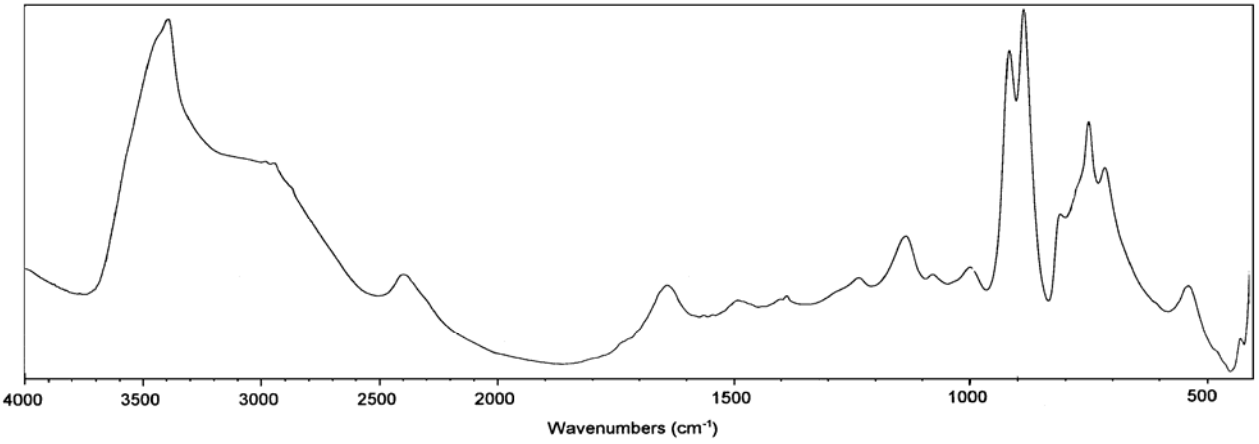
Cont.

I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*	I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*	I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*
<1	1.8837	1.8852	4	-2	-2			1.2962	4	-2	-4	4	0.98808	0.98807	6	0	2
3	1.8792	1.8802	4	-3	-1			1.2960	4	-4	2			0.98794	7	2	-3
23	1.8722	1.8725	1	3	-2			1.2951	2	-4	-3	4	0.98290	0.98310	4	-6	3
6	1.8595	1.8598	4	0	0	3	1.2902	1.2904	3	4	-2			0.98304	1	7	-1
16	1.8463	1.8473	1	-4	1	2	1.2787	1.2789	2	-6	0	2	0.97294	0.97277	8	-1	-4
3	1.8343	1.8320	2	1	-3	11	1.2739	1.2725	1	3	-4	5	0.97098	0.96987	8	-3	-4
1	1.8290	1.8295	2	-1	-3	7	1.2661	1.2672	-6	4	0	6	0.96703	0.96523	2	-7	3
5	1.8181	1.8193	2	2	1			1.2652	3	2	2			0.96616	0	7	1
14	1.8133	1.8132	2	3	-1	4	1.2559	1.2564	0	3	-4	<1	0.96309	0.96344	8	-5	0
12	1.8046	1.8055	3	-4	0			1.2562	1	-1	4	4	0.95133	0.95104	3	-4	-5
28	1.7968	1.7984	2	-4	1			1.2550	5	-5	-2	1	0.95084	0.95094	-7	0	5
		1.7969	2	-4	-1	8	1.2510	1.2513	4	3	0	4	0.95015	0.95035	7	-6	1
18	1.7776	1.7789	0	4	0			1.2500	1	-6	1			0.95004	3	1	-6
		1.7778	3	2	-2			1.2501	1	-2	4			0.94936	9	-3	-2
		1.7773	1	-1	-3	7	1.24924	1.24847	1	-5	-2	1	0.93920	0.93934	4	1	-6
42	1.7607	1.7630	0	0	3	1	1.24763	1.24760	4	3	-3	<1	0.93677	0.93732	3	-1	-6
		1.7600	1	3	1	12	1.23895	1.23920	3	-6	1			0.93723	3	-8	-1
3	1.7590	1.7580	3	-4	-1			1.23845	3	-6	-1	4	0.93677	0.93730	9	-4	-2
8	1.7507	1.7516	2	-3	2			1.23821	5	-2	-4	3	0.92577	0.92509	2	5	-5
7	1.7253	1.7253	2	3	0	4	1.23390	1.23428	4	-6	0	1	0.92106	0.92135	2	3	4
10	1.7080	1.7084	0	2	-3	1	1.22443	1.22462	6	1	-1	1	0.91793	0.91746	1	-5	5
6	1.6988	1.6989	5	-2	-1			1.22445	1	0	4	2	0.91589	0.91602	6	4	-1
6	1.6696	1.6703	2	-2	-3	6	1.22119	1.22081	5	-5	1			0.91541	7	-5	2
1	1.6675	1.6667	2	1	2	6	1.21816	1.21868	4	-6	-1	3	0.91492	0.91477	4	-2	-6
15	1.6625	1.6632	3	-4	1			1.21769	1	-5	3	3	0.91379	0.91371	7	-1	2
27	1.6526	1.6527	4	1	0	1	1.21573	1.21598	7	-2	-2	2	0.90997	0.91041	9	-5	-2
32	1.6436	1.6443	5	-1	-2	4	1.21004	1.20969	6	-5	-1			0.90992	3	2	4
15	1.6358	1.6362	4	-4	-1	7	1.20855	1.20852	5	1	1	1	0.90465	0.90451	0	8	-1
9	1.6319	1.6322	3	-2	2	4	1.20641	1.20664	1	5	1	4	0.90373	0.90358	5	4	1
15	1.6303	1.6309	4	-4	0	3	1.18739	1.18742	2	5	0	2	0.90276	0.90274	6	-8	0
		1.6289	-5	2	2	2	1.18599	1.18594	0	6	0			0.90261	8	-5	-4
10	1.6252	1.6255	3	-1	2			1.18595	4	-6	1	1	0.89452	0.89452	0	2	-6
		1.6247	0	3	2							<1	0.89110	0.89068	9	-5	-3

Infrared absorption spectrum (drift) of $Ca(H_2AsO_4)_2$ from Jáchymov.



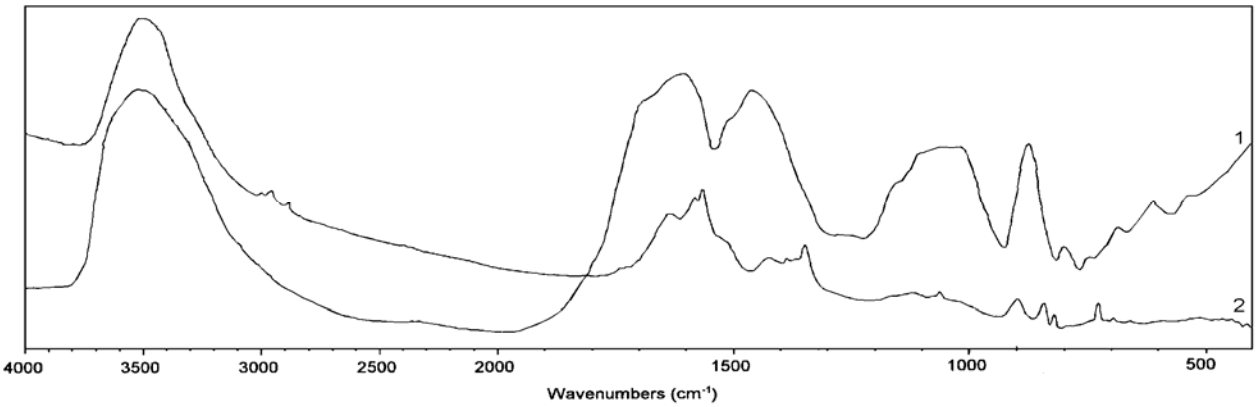
Infrared absorption spectrum (KBr tablet) of $Ca(H_2AsO_4)_2$ from Jáchymov.



X-ray powder diffraction pattern of "pseudo-voglite" from Jáchymov.

I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
2	17.819	5	6.060	30	4.027	17	3.211	11	2.4753
25	14.362	7	5.769	25	4.006	3	3.180	10	2.4239
11	13.059	19	5.415	9	3.959	19	3.084	20	2.4121
54	10.810	38	5.398	7	3.873	11	3.064	3	2.3416
76	9.657	11	5.210	15	3.800	14	3.052	<1	2.3037
56	8.835	12	5.125	11	3.777	7	2.982	4	2.2167
3	8.328	100	4.829	53	3.702	34	2.872	3	2.2002
21	8.041	16	4.783	10	3.667	5	2.825	17	2.1147
6	7.761	8	4.665	3	3.591	10	2.807	4	2.0936
72	7.602	13	4.584	8	3.537	6	2.783	4	2.0015
93	7.178	13	4.530	3	3.513	12	2.698	1	1.9454
25	7.090	20	4.409	4	3.481	11	2.645	9	1.9270
44	6.830	15	4.329	10	3.347	3	2.609	4	1.8910
38	6.517	28	4.234	8	3.258	6	2.580	5	1.8593
46	6.178	15	4.134	19	3.225	13	2.510	2	1.7601

Infrared absorption spectra (KBr tablet) of "pseudo-voglite" and voglite from Jáchymov



1 - Voglite, Jáchymov. Čejka et al. [16]
2 - "Pseudo-voglite" - $Ca_5Cu(UO_2)_4(CO_3)_6(OH)_8$. 4 H_2O, Jáchymov. This study

"Pseudo-voglite" $Ca_5Cu(UO_2)_4(CO_3)_6(OH)_8$. 4 H_2O

It forms platy skeletal crystals or granular aggregates of a bright green colour. The mineral adheres to surface of a thin fracture cutting a small carbonate vein with uraninite, pyrite and chalcopyrite. It does not fluoresce in UV light. "Pseudo-voglite" represents the oldest mineral in the succession: "pseudo-voglite" - liebigite - gypsum - schröckingerite.

EDX, WDX		major elements: U, Ca, Cu, CO_3^{2-}	minor elements:
IR [cm^{-1}] (KBr)		735,849,904,1064,1119,1346,1384,1421, 1562,1578,1630,2852,2922,2962,3447	
References		16, 30, 42, 56, 163	

Results of 3 analyses gave, when averaged, the following results: Ca 9.26, Cu 3.52, U 48.53, O 29.97, C 3.52, total 94.81 wt. %, and the proposed empirical formula (based on 39 O):

$Ca_{4.81}Cu_{1.15}(UO_2)_{4.212}(CO_3)_{6.12}(OH)_{8.19}$. 3.97 H_2O

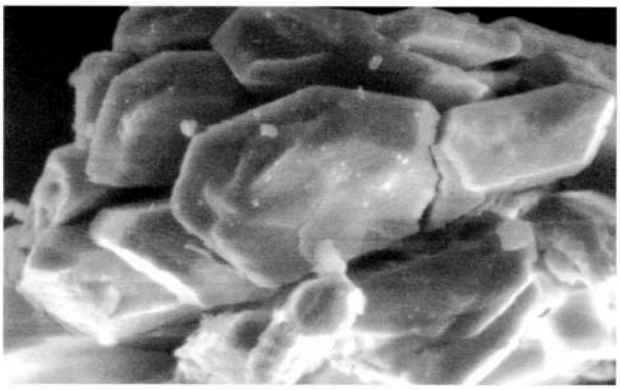
leads to simplified formula:

$Ca_5Cu(UO_2)_4(CO_3)_6(OH)_8$. 4 H_2O

or

$Ca_5Cu(UO_2)_4(CO_3)_6O_4$. 8 H_2O

The mineral was identified in samples from the Klement vein (specimen number: J-363).



Aggregate of pseudohexagonal crystals of "pseudo-voglite". Magnification 1000

The phase: $Ca_2Cu(UO_2)_2(CO_3)_2O_3$. 3 H_2O

It forms imperfect crystals grouped into fan-shaped aggregates. It has yellow-green colour and vitreous lustre. It is very brittle. Aggregates are situated in fractures

(covered by limonite) in a rock. The sample was found in material from the Fluther vein, Elias mine. Phase $Ca_2Cu(UO_2)_2(CO_3)_2O_3$. 3 H_2O appears to be associated with no other minerals. Specimen number: 45172 (National museum, Prague).

Results of 3 analyses gave, when averaged, the following results: Ca 7.10, Cu 6.42, U 50.50, O 26.11, C 2.18, total 92.31 wt. %, and the proposed empirical formula (based on 17 O):

$$Ca_{1.85}Cu_{1.05}(UO_2)_{2.21}(CO_3)_{1.89}(OH)_{6.43}$$

leads to simplified formula:

$$Ca_2Cu(UO_2)_2(CO_3)_2(OH)_6$$

or

$$Ca_2Cu(UO_2)_2(CO_3)_2O_3 \cdot 3\ H_2O$$

The latter formula corresponds to that of voglite (this issue) with 3 water molecules.

The phase: Ca-Cu-(UO_2)-(CO_3)-H_2O

Phase forms crystalline to glassy crusts, 1-2 mm thick, rimming crystalline aggregates of rösslerite. It is of green colour. It regularly inter-grows with glassy yellow-green amorphous phases and is rimmed with pale green to whitish botryoidal aggregates of cuprosklodowskite. Usually it is associated with liebigite, voglite, rösslerite, brassite, cuprosklodowskite, gypsum, and zellerite. Specimen number: 244J.

The phase was found in the vein No. 3.

EDX, WDX		major elements: U, Ca, Cu, CO_3^{2-}	minor elements: Mg, Si

"Pseudo-johannite" Cu-UO_2-SO_4-H_2O

"Pseudo-johannite" forms brittle and soft aggregates or coatings with an uneven or botryoidal surface, which are composed of very fine crystals. The colour is grey olive and the mineral is not lustrous. The aggregates are deposited directly on strongly weathered uraninite.

"Pseudo-johannite" occurs in paragenesis with johannite, uranopilite and gypsum on specimen from the Werner shaft; specimen number: J-357.

EDX, WDX		major elements: Cu, U, S	minor elements:
Therm. analysis [°C, wt. %]		20-160 9.0 (loss of H_2O)	
IR [cm^{-1}]		Drift:488,551,583,626,674,758,830,877, 1078,1156,1627,2855,2929,3220,3315, 3378,3460	
		KBr:475,497,583,625,674,831,874,1077, 1151,1457,1560,1627,3375,3453	
References		11, 166, 167, 168, 201, 252	

X-ray powder diffraction pattern of phase $Ca_2Cu(UO_2)_2(CO_3)_2O_3$. 3 H_2O from Jáchymov.

I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
20	10.994	11	7.792	15	5.835	26	4.079	33	3.043
16	10.678	18	7.597	46	5.684	43	3.410	30	3.014
29	9.419	13	7.164	13	5.024	21	3.375	16	2.995
96	9.094	100	6.250	38	4.967	21	3.339	28	2.801
46	8.763	13	6.034	24	4.304	11	3.305	32	2.516
19	8.420								

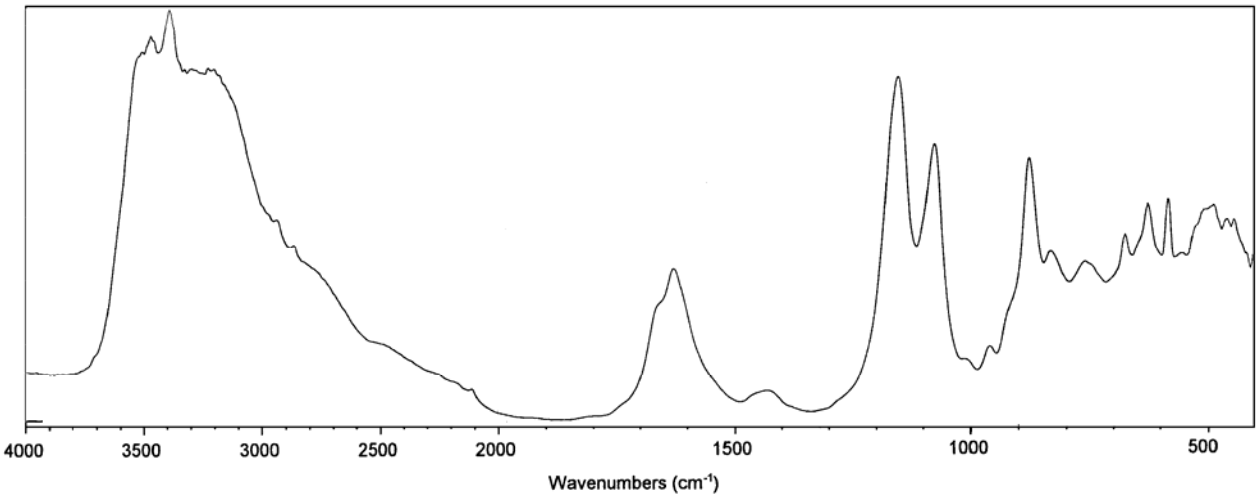
X-ray powder diffraction pattern of phase Ca-Cu-(UO_2)-(CO_3)-H_2O from Jáchymov.

I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
100	10.994	20	7.253	7	5.711	19	4.197	21	3.036
53	9.543	15	7.114	15	5.485	41	3.983	19	2.779
12	9.191	13	6.794	26	5.369	22	3.921	10	2.4250
56	8.716	39	6.428	11	5.135	28	3.664	12	2.0875
22	7.935	27	6.156	52	4.765	14	3.173		

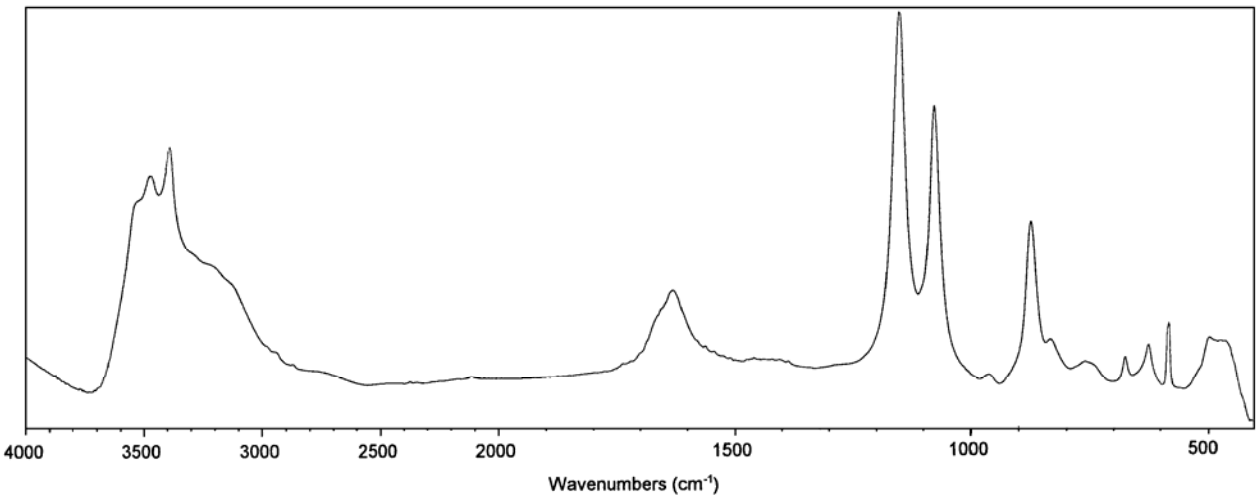
X-ray powder diffraction pattern of "pseudo-johannite" from Jáchymov.

I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
5	13.206	7	3.876	7	2.846	5	2.2131	3	1.8528
100	9.134	6	3.766	15	2.783	14	2.1551	10	1.8440
6	8.332	3	3.650	10	2.693	5	2.1376	3	1.8249
12	7.732	8	3.562	16	2.666	10	2.1064	8	1.7893
30	7.110	4	3.542	4	2.618	5	2.0878	9	1.7460
2	6.141	18	3.448	7	2.583	5	2.0731	14	1.7193
21	5.527	13	3.373	2	2.562	5	2.0519	4	1.6846
7	4.935	7	3.325	4	2.521	5	2.0336	4	1.6757
3	4.731	12	3.301	13	2.4980	7	1.9885	7	1.6455
79	4.573	14	3.158	4	2.4561	6	1.9659	3	1.6345
5	4.416	5	3.121	3	2.4226	5	1.9379	3	1.6178
13	4.209	15	3.082	6	2.3953	8	1.9174	6	1.5946
5	4.170	23	3.048	16	2.3670	3	1.9051	4	1.5836
9	4.046	11	2.950	4	2.3420	1	1.8889	3	1.5761
2	3.967	22	2.866	14	2.2883	5	1.8772	3	1.5442

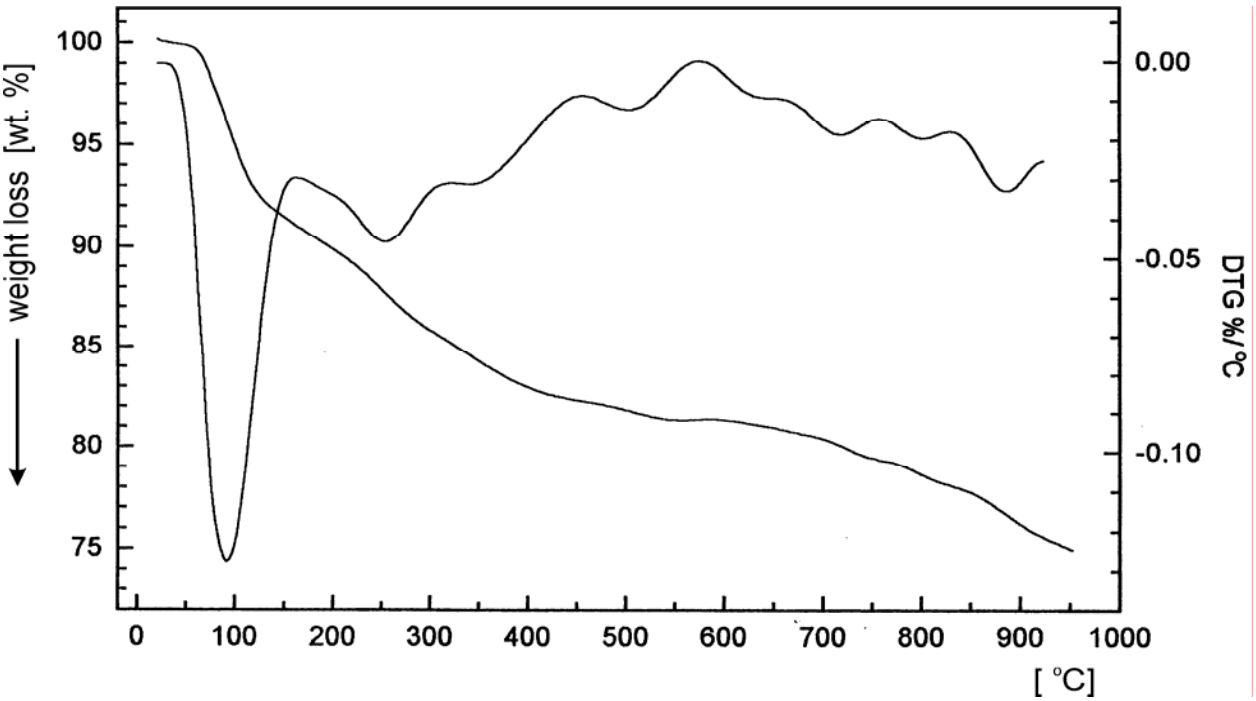
Infrared absorption spectrum (drift) of "pseudo-johannite" from Jáchymov.



Infrared absorption spectrum (KBr tablet) of "pseudo-johannite" from Jáchymov

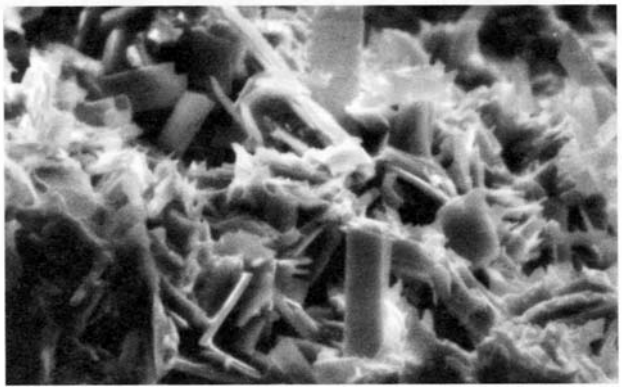


Thermogravimetric (TG,DTG) curves of "pseudo-johannite" from Jáchymov



X-ray powder diffraction pattern of Fe-AsO_4-H_2O(1) from Jáchymov.

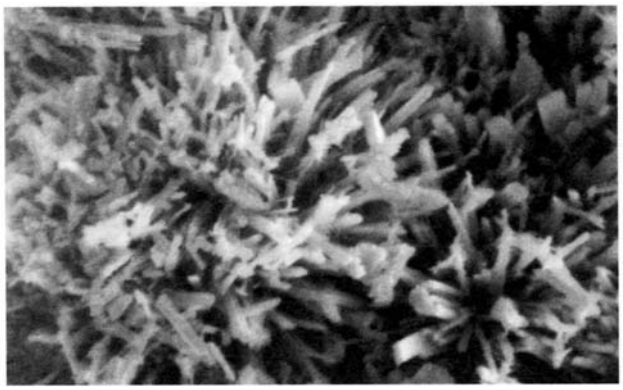
I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
100	12.480	14	4.836	8	3.452	6	2.842	4	2.3391
10	8.401	27	4.758	10	3.385	8	2.804	10	2.3209
31	6.473	12	4.527	20	3.364	4	2.780	6	2.2913
54	6.266	14	4.461	8	3.331	3	2.760	8	2.2656
9	5.963	36	4.380	17	3.299	8	2.717	5	2.1483
6	5.826	17	4.208	5	3.246	12	2.639	1	2.1299
11	5.763	22	4.149	19	3.182	6	2.619	3	2.0418
16	5.603	23	4.102	8	3.139	18	2.590	2	2.0282
3	5.492	24	4.014	4	3.103	11	2.563	5	1.9706
15	5.433	9	3.857	14	3.066	7	2.530	6	1.7259
21	5.307	27	3.808	9	3.019	18	2.506	4	1.7068
4	5.253	5	3.767	13	2.994	5	2.4674	5	1.6857
5	5.137	20	3.719	11	2.957	7	2.4473	7	1.5911
12	5.076	7	3.606	15	2.924	2	2.3912	2	1.5714
9	5.012	11	3.564	10	2.892	9	2.3791	3	1.5510
8	4.952	7	3.501	4	2.863				



Prismatic, randomly oriented crystals of "pseudo-johannite". Magnification 1000

The phase: Fe-AsO_4-H_2O (1)

The phase Fe-AsO_4-H_2O(1) (sample: J-244) forms small white, beige, or light greyish earthy-appearing aggregates composed of minute acicular crystals, deposited on a matrix of coarse, rusty-coloured gypsum. The aggregates are either relatively compact or soft and coherent.



Aggregate of minute acicular crystals of the phase Fe-AsO_4-H_2O (1). Magnification 900

The phase Fe-AsO_4-H_2O(1) is in paragenesis with morenosite, nickelhexahydrite, an unknown manganese sulphate, krautite and gypsum.

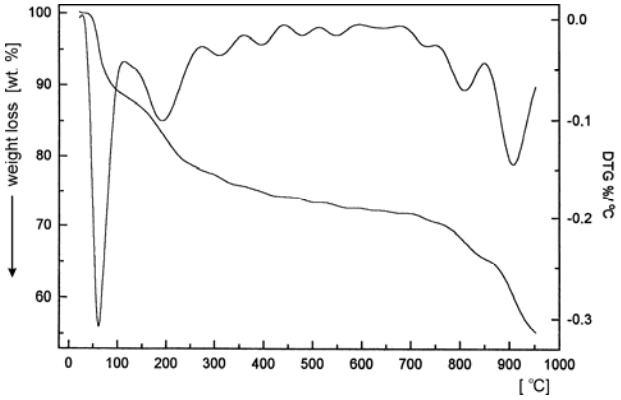
The specimens were collected in the Geschieber vein.

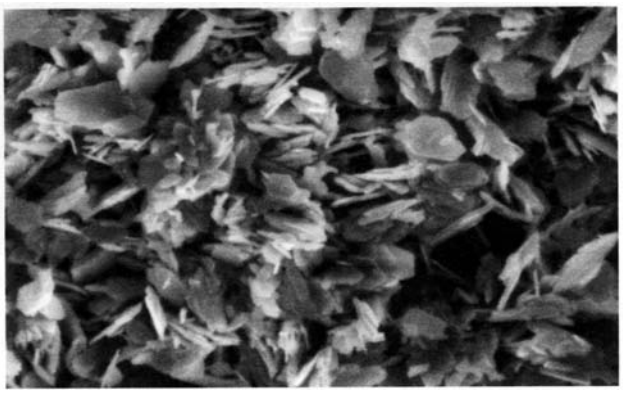
EDX, WDX		major elements: Fe, As	minor elements:
References		66, 67, 261, 290	

The phase: Fe-AsO_4-H_2O (2)

The phase Fe-AsO_4-H_2O(2) (sample: J-434) forms aggregates very similar to those of the phase Fe-AsO_4-H_2O(1) - small white, beige, or light greyish earthy-appearing aggregates composed of minute acicular crystals, deposited on a matrix of coarse, rusty-coloured gypsum.

Thermogravimetric (TG,DTG) curves of "Fe-AsO_4-H_2O(2)" from Jáchymov





Aggregate of minute tabular crystals of the phase Fe-AsO_4-H_2O (2). Magnification 1000

The phase Fe-AsO_4-H_2O(2) is in paragenesis with morenosite, nickelhexahydrite, an unknown manganese sulphate, krautite and gypsum.

The specimens were collected in the Geschieber vein.

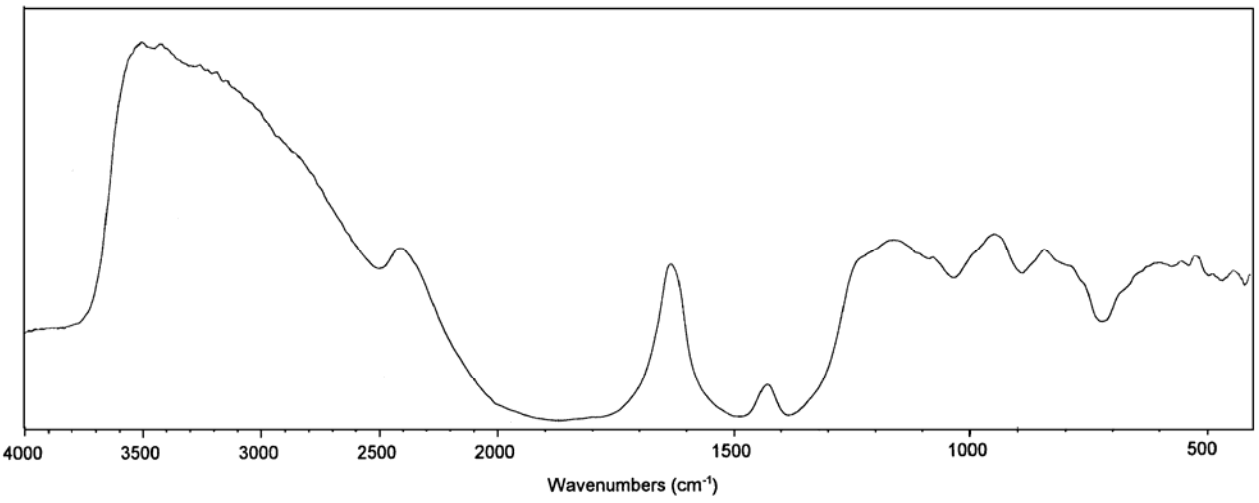
Self-indexing [291] procedure applied to measured X-ray powder data provided orthorhombic, probably primitive cell (see table below).

Lattice par. [Å]	a= 10.676(1)	b= 19.027(3)	c= 10.010(1)
Therm. analysis [°C, wt. %]	20-110 11.3 (partial loss of H_2O), 110-270 10.7 (partial loss of H_2O)		
IR [cm^{-1}]	Drift:406,423,443,487,523,550,598,839, 946,1078,1160,1428,1632,2400,3139, 3183,3249,3408,3489,3890,3938,3968		
	KBr: 430,456,476,560,672,824,869,960, 1104,1634,2389,3448		
EDX, WDX	major elements: Fe, As	minor elements:	
References	66,67,261,290		

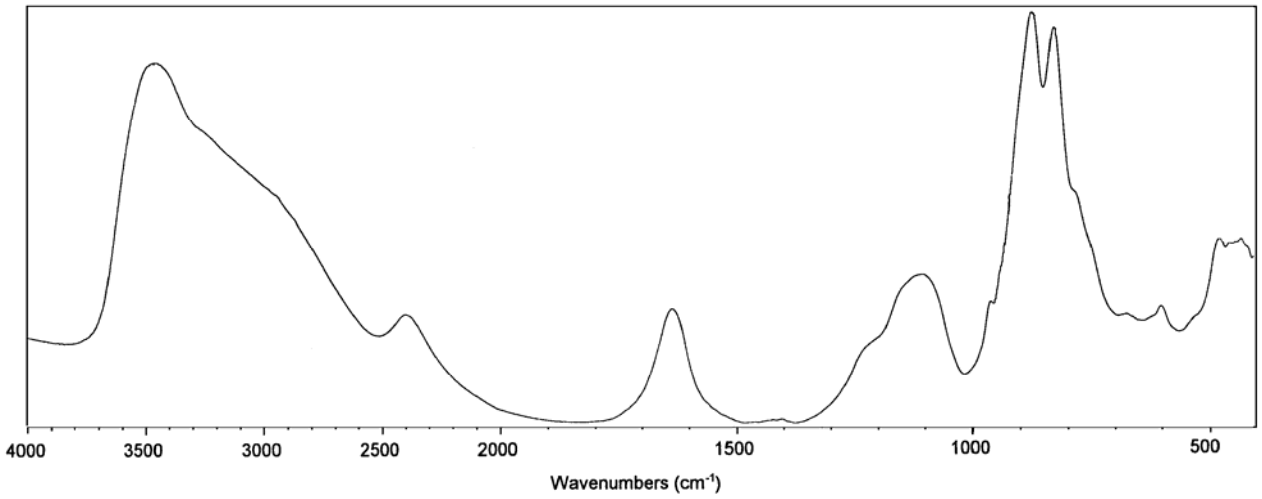
X-ray powder diffraction pattern of Fe-AsO_4-H_2O(2) from Jáchymov.

I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*	I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*	I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*
100	9.497	9.522	0	2	0	11	2.517	2.516	3	5	1	5	1.6832	1.6834	1	11	1
85	9.308	9.318	1	1	0	5	2.4895	2.4896	4	2	1	6	1.6773	1.6782	3	10	0
24	6.811	6.822	1	1	1	10	2.4367	2.4371	1	0	4	4	1.6703	1.6703	6	1	2
13	5.790	5.796	1	2	1	4	2.4161	2.4173	1	1	4	3	1.6534	1.6542	4	7	3
23	5.454	5.455	1	3	0	9	2.3937	2.3947	2	6	2	2	1.6486	1.6486	1	0	6
13	5.335	5.341	2	0	0	13	2.3560	2.3556	4	0	2	4	1.6359	1.6354	3	7	4
9	5.004	5.007	0	0	2	4	2.3374	2.3377	4	1	2	4	1.6249	1.6245	5	0	4
11	4.788	4.791	1	3	1	4	2.3299	2.3315	1	7	2	1	1.6170	1.6162	1	11	2
6	4.654	4.657	2	2	0	5	2.3063	2.3072	3	5	2	14	1.5936	1.5941	1	7	5
5	4.569	4.574	2	1	1	6	2.2867	2.2865	4	2	2	7	1.5872	1.5871	2	1	6
9	4.529	4.534	1	0	2	15	2.2681	2.2676	4	4	1	3	1.5803	1.5814	6	4	2
2	4.407	4.410	1	1	2	4	2.2085	2.2082	4	3	2	2	1.5714	1.5708	2	2	6
35	4.221	4.223	2	2	1	7	2.1684	2.1690	1	4	4	3	1.5647	1.5649	6	1	3
6	4.091	4.093	1	2	2	8	2.1074	2.1078	0	7	3	9	1.5505	1.5517	3	8	4
10	3.988	3.987	1	4	1	4	2.0765	2.0761	5	1	1	2	1.5142	1.5146	5	8	2
16	3.782	3.783	2	3	1	6	2.0687	2.0689	0	9	1	2	1.5006	1.5001	5	7	3
18	3.650	3.652	2	0	2	4	2.0512	2.0523	1	5	4	2	1.4690	1.4692	2	5	6
39	3.586	3.587	2	1	2	4	2.0418	2.0424	4	6	0	2	1.4600	1.4606	5	0	5
6	3.497	3.499	3	1	0	3	2.0335	2.0357	3	1	4	4	1.4569	1.4573	2	10	4
14	3.448	3.449	0	4	2	2	2.0240	2.0240	5	3	0	4	1.4420	1.4422	7	2	2
4	3.408	3.410	2	2	2	8	2.0029	2.0029	4	5	2	2	1.4386	1.4390	5	9	2
6	3.377	3.376	1	5	1	10	1.9844	1.9838	5	3	1	4	1.4243	1.4249	6	8	0
20	3.347	3.348	2	4	1	10	1.9597	1.9605	2	7	3	3	1.4163	1.4158	7	5	0
24	3.302	3.303	3	1	1	5	1.9484	1.9484	3	3	4	3	1.4108	1.4110	4	1	6
13	3.281	3.282	1	4	2	7	1.9409	1.9402	3	8	1	3	1.4030	1.4027	2	9	5
18	3.161	3.163	3	2	1	11	1.9304	1.9312	3	6	3	3	1.3947	1.3949	7	4	2
16	3.147	3.150	0	2	3	3	1.8812	1.8807	3	4	4	3	1.3843	1.3836	7	1	3
26	3.104	3.104	3	3	0	2	1.8713	1.8712	4	7	1	2	1.3781	1.3779	2	1	7
12	3.021	3.021	1	2	3	1	1.8627	1.8624	5	5	0	4	1.3708	1.3705	6	8	2
27	2.963	2.965	3	3	1	6	1.8425	1.8439	2	6	4	4	1.3639	1.3639	3	6	6
10	2.913	2.915	1	5	2	10	1.8312	1.8310	5	5	1	5	1.3596	1.3597	6	7	3
15	2.847	2.847	1	3	3	4	1.8151	1.8156	5	4	2	2	1.3290	1.3291	1	12	4
22	2.799	2.799	2	1	3	4	1.8034	1.8031	3	5	4	3	1.3222	1.3229	8	0	1
9	2.732	2.732	0	4	3	7	1.7894	1.7908	5	1	3	3	1.3181	1.3186	7	7	1
12	2.712	2.713	2	2	3	5	1.7801	1.7802	4	7	2	2	1.3108	1.3117	5	1	6
7	2.643	2.644	4	1	0	5	1.7466	1.7482	1	5	5	2	1.2816	1.2810	6	4	5
8	2.600	2.600	3	5	0	6	1.7254	1.7243	0	8	4	2	1.2749	1.2753	3	8	6
11	2.556	2.556	4	1	1	1	1.6903	1.6889	6	3	1						

Infrared absorption spectrum (Drift) of "Fe-AsO_4-H_2O(2)" from Jáchymov.



Infrared absorption spectrum (KBr tablet) of "Fe-AsO_4-H_2O(2)" from Jáchymov.



X-ray powder diffraction pattern of Mg-AsO_4-H_2O from Jáchymov

I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*	I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*	I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*
100	16.216	16.209	0	0	2	19	2.960	2.962	1	2	3	6	1.9379	1.9382	2	1	13
49	8.109	8.105	0	0	4	14	2.876	2.873	2	0	8	5	1.9086	1.9093	0	2	15
16	7.911	7.904	0	1	1	15	2.781	2.782	1	2	5	6	1.8646	1.8650	0	4	7
9	7.277	7.281	1	0	2	27	2.771	2.771	0	1	11	5	1.8564	1.8568	1	0	17
5	6.502	6.507	1	0	3	22	2.702	2.702	0	0	12	7	1.8505	1.8510	1	2	14
25	5.744	5.747	1	0	4	9	2.674	2.676	1	2	6	6	1.8014	1.8010	0	0	18
2	5.407	5.403	0	0	6	14	2.564	2.564	1	0	12	10	1.7769	1.7758	4	1	1
2	5.072	5.074	1	0	5	7	2.536	2.537	0	2	10	8	1.7681	1.7670	3	2	6
22	4.707	4.705	1	1	0	10	2.498	2.498	1	1	11	5	1.7321	1.7336	1	3	12
20	4.653	4.657	1	1	1	12	2.4509	2.4523	1	2	8	5	1.7274	1.7272	0	2	17
10	4.505	4.503	0	1	6	17	2.3850	2.3846	1	0	13	3	1.6968	1.6977	3	2	8
16	4.312	4.314	1	1	3	21	2.3425	2.3428	1	1	12	3	1.6918	1.6913	0	3	15
73	4.057	4.052	0	0	8	5	2.3159	2.3156	0	0	14	3	1.6585	1.6595	3	2	9
20	4.026	4.027	0	1	7	6	2.2572	2.2565	0	3	8	7	1.6469	1.6473	0	2	18
18	3.952	3.952	0	2	2	10	2.2281	2.2274	1	0	14	7	1.6210	1.6209	0	0	20
16	3.806	3.808	1	1	5	8	2.2029	2.2034	1	1	13	9	1.6170	1.6175	1	3	14
9	3.628	3.629	0	1	8	7	2.1761	2.1773	1	3	4	7	1.6040	1.6040	1	1	19
14	3.549	3.548	1	1	6	5	2.1282	2.1270	2	0	13	3	1.5549	1.5548	1	2	18
3	3.451	3.450	2	0	5	6	2.0889	2.0890	1	0	15	5	1.5312	1.5297	0	4	14
24	3.300	3.301	1	1	7	12	2.0777	2.0776	1	1	14	6	1.5167	1.5168	1	0	21
43	3.244	3.242	0	0	10	7	2.0279	2.0261	0	0	16	4	1.4923	1.4926	1	2	19
6	3.068	3.067	1	2	1	4	2.0121	2.0133	0	2	14	5	1.4498	1.4500	1	0	22
7	3.015	3.012	1	0	10	7	1.9732	1.9741	3	1	8						

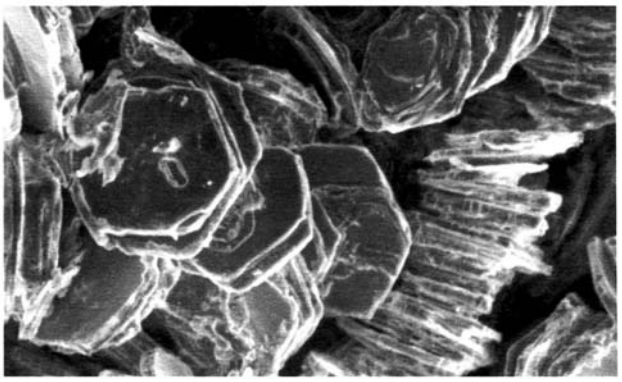
The phase: Mg-AsO_4-H_2O

The phase Mg-AsO_4-H_2O (sample: J-0495/3) forms minute, thin tabular crystals (size: up to 1 mm), seemingly of hexagonal habit, transparent or white. It has a vitreous to pearly lustre. The phase is associated, and in part intergrown, with thenardite.

Phase Mg-AsO_4-H_2O is partially soluble in H_2O.

Self-indexing [291] procedure applied to measured X-ray powder data provided hexagonal, probably primitive cell (see table below).

Lattice par. [Å]		a = 9.411(1)		c =32.418(3)
		Hexagonal, V =2486.5(6)		
EDX, WDX		major elements: Mg, As		minor elements: Na
References		107, 145, 210		

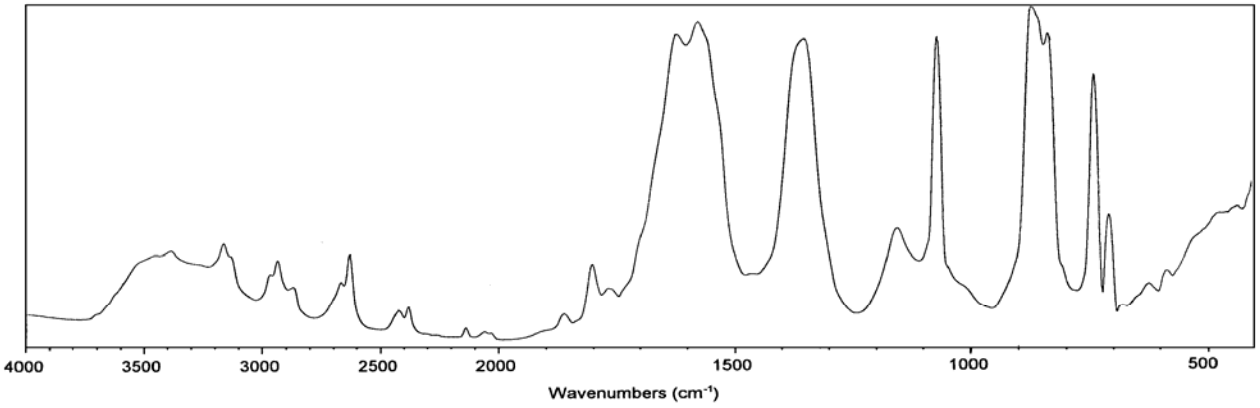


Hexagonal crystals of the phase Mg-AsO_4-H_2O. Magnification 150

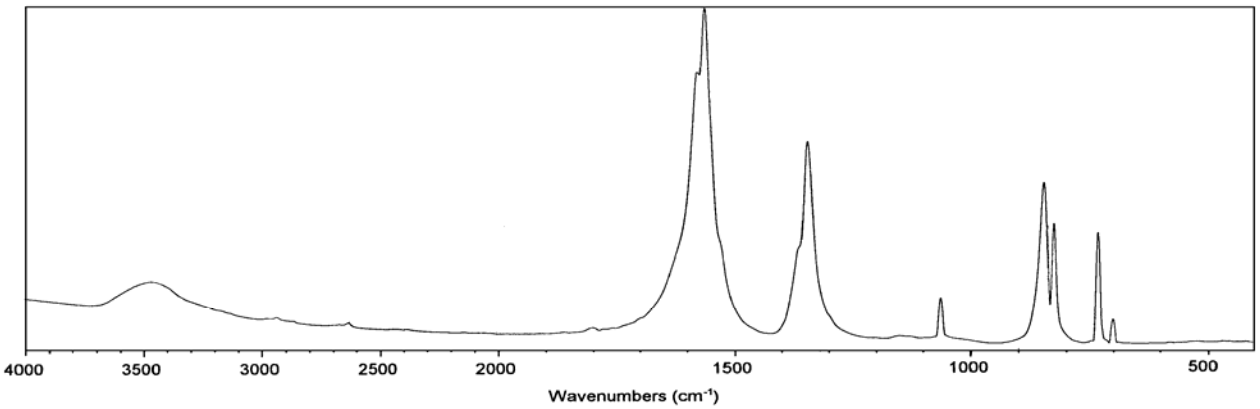
The phase: $Na_4(UO_2)(CO_3)_3$

The phase $Na_4(UO_2)(CO_3)_3$ forms minute earthy aggregates on the order of 100 μm in size. They are deposited on wall rock or even on continuous coating of dust.

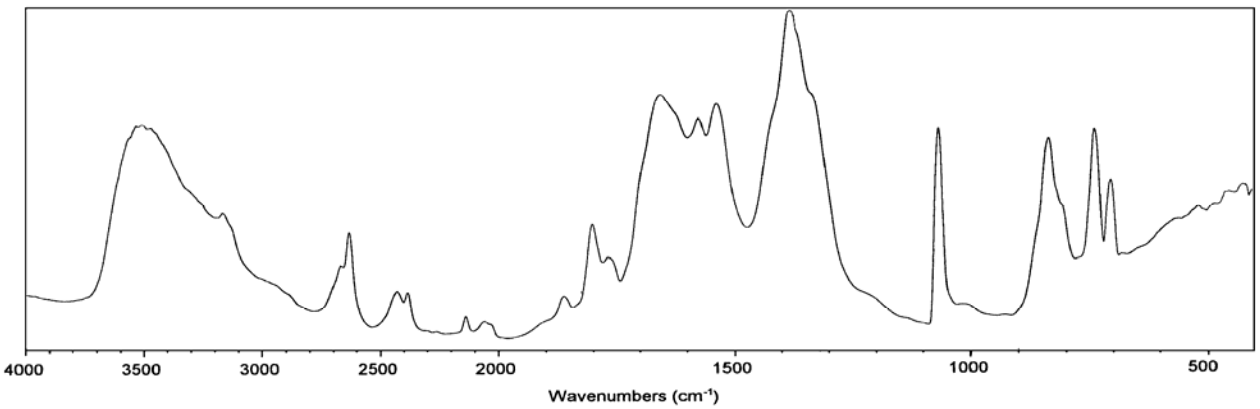
Infrared absorption spectrum (drift) of $Na_4(UO_2)(CO_3)_3$ from Jáchymov.



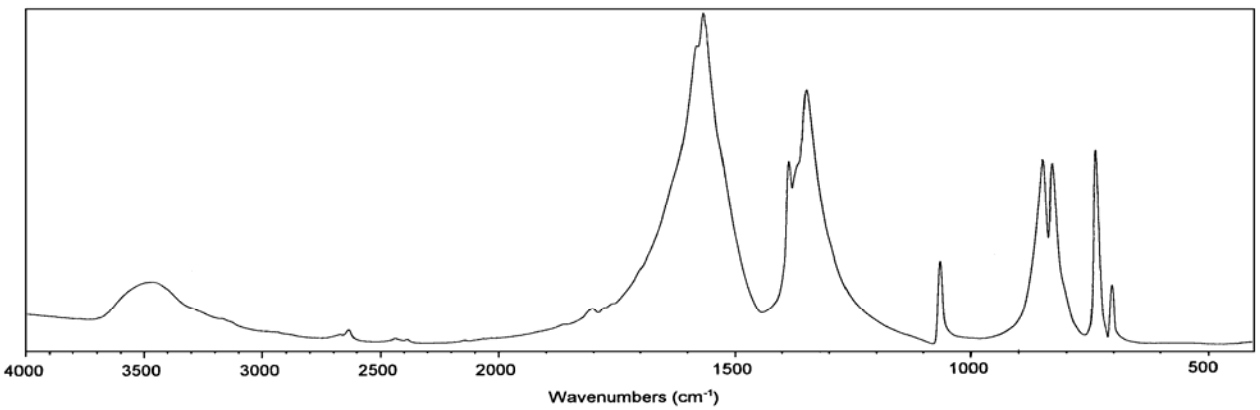
Infrared absorption spectrum (KBr tablet) of $Na_4(UO_2)(CO_3)_3$ from Jáchymov.



Infrared absorption spectrum (drift) of synthetic $Na_4(UO_2)(CO_3)_3$.



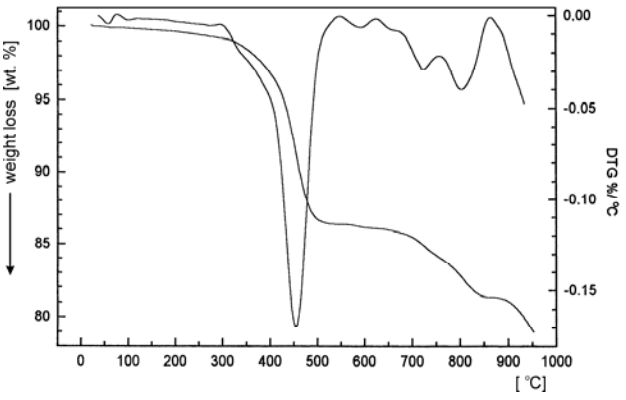
Infrared absorption spectrum (KBr tablet) of synthetic $Na_4(UO_2)(CO_3)_3$



X-ray powder diffraction pattern of $Na_4(UO_2)(CO_3)_3$ from Jáchymov.

		triclinic indexing				hexagonal indexing			
I_{rel}	d_{obs}	*h*	*k*	*l*	d_{calc}	*h*	*k*	*l*	d_{calc}
8	23.568	0	1	0	23.104				
6	16.126	-1	1	0	16.164	0	1	0	16.126
2	12.257								
73	8.071	-2	2	0	8.082	2	0	0	8.063
15	7.838	-2	1	0	7.762				
52	5.105	0	1	-1	5.132				
52	5.043	1	1	-1	5.048				
54	4.987	-3	1	0	4.988	2	0	2	5.013
100	4.654	1	-2	1	4.650	2	2	0	4.655
45	4.034	-3	3	1	4.032	0	4	0	4.032
3	3.917	-2	7	0	3.920	1	1	3	3.879
30	3.457	0	4	1	3.466	2	1	3	3.496
31	3.420	-3	8	0	3.417	4	0	2	3.411
29	3.384	-4	1	1	3.386	4	1	1	3.393
64	3.229	-4	8	0	3.229	0	5	0	3.225
39	3.047	4	1	-1	3.043	2	4	0	3.048
12	3.021	1	4	1	3.014	3	3	1	3.016
17	2.997	-2	9	0	2.999	0	2	4	2.975
22	2.973	-2	7	1	2.969				
32	2.784	-1	7	1	2.784	3	3	2	2.793
19	2.774	-3	8	1	2.774				
27	2.765	2	6	0	2.768				
23	2.746	-4	8	1	2.747	0	3	4	2.750
18	2.735	1	5	1	2.734				
22	2.726	2	6	-1	2.729	4	1	3	2.715
79	2.687	3	-9	1	2.687	6	0	0	2.688
7	2.668	-2	10	0	2.674				
12	2.635	4	3	-1	2.638	2	2	4	2.637
6	2.618	-5	8	1	2.617				
14	2.549	-4	9	1	2.548	0	0	5	2.560
12	2.520	1	8	-1	2.520	1	0	5	2.529
16	2.4904	-4	11	0	2.4906	4	2	3	2.4800
66	2.3262	-6	9	1	2.3260	4	4	0	2.3276
14	2.2448	4	2	1	2.2450	2	2	5	2.2434
43	2.2349					6	2	0	2.2363
7	2.2258	0	-7	2	2.2258	3	3	4	2.2279
10	2.2050	6	-5	1	2.2044	6	2	1	2.2029
7	2.1950	-3	6	2	2.1939	4	4	2	2.1875
6	2.1853	-7	3	0	2.1856				
22	2.1289	2	-8	2	2.1331	6	1	3	2.1307
17	2.1246	4	3	-2	2.1238				
18	2.1164	3	-7	2	2.1153	0	1	6	2.1151
14	2.1078	4	3	1	2.1081	1	7	1	2.1068
16	2.0985	-4	7	2	2.0983				
6	2.0942								
17	2.0905	-3	7	2	2.0915				
16	2.0788	-7	10	1	2.0792	1	1	6	2.0797
24	2.0659	3	-8	2	2.0657	4	5	0	2.0647
1	2.0605	2	9	0	2.0604	6	0	4	2.0582
15	2.0403	-5	12	1	2.0390	5	4	1	2.0384
18	2.0142	-6	6	2	2.0158	2	1	6	2.0138
11	1.9356	0	6	2	1.9361	6	3	2	1.9365
7	1.9234	-8	10	1	1.9234	0	8	2	1.9227
10	1.9166	-7	12	1	1.9165	1	5	5	1.9183
12	1.9099	-2	12	1	1.9102	7	1	3	1.9100
15	1.8984	3	7	-2	1.8981				
15	1.8788					4	4	4	1.8824
7	1.8743	3	-14	1	1.8733	7	0	4	1.8697
2	1.8629	6	4	-1	1.8638	5	5	0	1.8621
8	1.8605	-6	9	2	1.8607	4	5	3	1.8586
4	1.8545	7	1	0	1.8535	0	6	5	1.8538
25	1.8481	4	6	-2	1.8470	3	2	6	1.8482
5	1.8313	-7	13	1	1.8308	6	4	1	1.8308
10	1.8200	-4	10	2	1.8203	5	2	5	1.8181
7	1.8139	0	11	1	1.8138	7	3	0	1.8143
15	1.7893	-9	9	1	1.7897	2	7	3	1.7887
9	1.7848	-6	14	1	1.7851				
8	1.7823	-3	15	0	1.7825	2	0	7	1.7835
13	1.7798	7	-13	1	1.7811	5	0	6	1.7794
17	1.7718	8	-9	1	1.7720	1	6	5	1.7736
12	1.7642	2	9	1	1.7646				
56	1.7579	5	-15	1	1.7580	3	3	6	1.7582
2	1.7491	4	-12	2	1.7491	4	2	6	1.7478
8	1.7450	5	-2	2	1.7450	7	3	2	1.7456
10	1.7348	1	2	-3	1.7349	4	5	4	1.7350
6	1.7268	-3	14	1	1.7262	8	1	3	1.7261
4	1.7090	6	-7	2	1.7088	5	5	3	1.7067
6	1.6902	-4	1	3	1.6912	1	9	0	1.6905
5	1.6228	1	-7	3	1.6234	4	1	7	1.6227
8	1.6133	4	3	2	1.6132				
10	1.6130	2	-14	2	1.6129	0	10	0	1.6126
3	1.5961	9	-11	1	1.5956				
5	1.5925	2	-7	3	1.5927	0	1	8	1.5924
8	1.5849	-6	13	2	1.5846	8	0	5	1.5838
10	1.5707	-6	1	3	1.5706	0	2	8	1.5696
6	1.5650	-7	13	2	1.5647	0	7	6	1.5654
7	1.5606	7	-6	2	1.5608	7	2	5	1.5614
5	1.5571	-1	11	2	1.5568	4	7	3	1.5569
6	1.5546	9	-13	1	1.5548				
10	1.5503	3	-6	3	1.5501	6	6	0	1.5517
11	1.5409	1	14	0	1.5413	6	6	1	1.5405
8	1.5342	2	-15	2	1.5340	0	3	8	1.5337
13	1.5303	3	-8	3	1.5298	10	1	0	1.5306
8	1.5267	0	14	-2	1.5265				
5	1.5225	-5	18	0	1.5227	4	8	0	1.5238
9	1.5177	-3	16	1	1.5177	8	1	5	1.5192
5	1.5109	2	-10	3	1.5107	6	0	7	1.5120
11	1.4877	6	-18	1	1.4877	4	0	8	1.4873
8	1.4794	1	10	-3	1.4788	3	7	5	1.4803
4	1.4723	-9	13	2	1.4722	6	3	6	1.4713

Thermogravimetric (TG,DTG) curves of synthetic $Na_4(UO_2)(CO_3)_3$.



The phase $Na_4(UO_2)(CO_3)_3$ was found in the same occurrence as andersonite and schröckingerite, but in the actual site it is free of associated minerals. It fluoresces weak yellow to yellow green in ultra-violet light.

Attempts in indexing the X-ray diffraction pattern using lattice parameters given in [230] was unsuccessful, because the natural sample $Na_4(UO_2)(CO_3)_3$, as well as the synthetic analogue, shows many additional diffractions.

The reflection at 16.126 Å observed by us indicates that the unit-cell dimensions have to be doubled at least if hexagonal symmetry is assumed. Even with this larger cell, 21% of reflection remain unindexed.

Lattice par. [Å]	1	a = 16.468(2)	b=27.578(3)	c = 5.222(2)
		α=94.155(2)	β=100.58(1)	γ=121.25(1) V=1952.9(8)
	2	a= 18.621(3)		c= 12.801(4)
				V=3844(2)
EDX, WDX		major elements: U, Na, C	minor elements:	
Therm. analysis [°C, wt. %]	3	20-550 13.6 (partial loss of CO_2)		
IR [cm^{-1}]	1	drift: 429,580,619,704,736,833,867, 1066,1151,1349,1573,1618,1765,1799, 2376,2416,2622,2658,2860,2927,2957, 3153,3377		
		KBr:703,735,827,846,1064,1345,1562, 1577,2622,2661,2927,2961,3452		
	3	drift:422,452,482,516,703,736,832,1064, 1381,1535,1574,1656,17656,1799,1858,2052, 2130,2377,2422,2622,2657,3155, 3520		
		KBr:702,734,825,844,1063,1345,1383,1561,1 576,3455		
References		230		

1 - phase $Na_4(UO_2)(CO_3)_3$, Jáchymov; this study. Unit-cell parameters for a triclinic cell and Z = 8 were suggested by indexing of the X-ray diffraction pattern.

2 - phase $Na_4(UO_2)(CO_3)_3$, Jáchymov; this study. Unit-cell parameters for a hexagonal cell and Z=8 were taken from [230], but the original parameter a=9.324 Å was doubled. 21% of diffractions could not be indexed using this model.

3 - synthetic $Na_4(UO_2)(CO_3)_3$. This study.

"Hydronium uranospinite" $(H_3O)_2(UO_2)_2(AsO_4)_2 . 8H_2O$

It occurs as clusters of minute flat crystals and as thin finely-crystalline crusts. The mineral is light yellow. It fluoresces yellow-white with a moderate intensity in UV light, sometimes with a yellow greenish shade. It occurs with zeunerite and anglesite along fractures of specimens containing uraninite and pyrite. The specimens were collected in the Eliáš mine and in the Schweitzer vein.

EDX, WDX		major elements: U, As	minor elements: Al, P, (Si)
References		271, 330, 331, 332	

"Pseudo-lindackerite" Cu-Ca-AsO_4-H_2O

It is probable that this phase was already studied in the past ([25], [60]), since some of its properties are very close to those reported for lindackerite.

"Pseudo-lindackerite" occurs in crystalline crusts or aggregates of whitish green, grey-green or apple green colour. The aggregates are composed of fine, brittle, lustrous and non-transparent crystals (the last property is in contrast to lindackerite). Individual orthorhombic crystals are up to 2 mm long and show a platy aggregation but other aggregates show predominance of lath-shaped crystals. The colour tends to a stronger variation in thin coatings.

The mineral features a regular paragenesis with lindackerite, geminite, lavendulan, strashimirite, olivenite, picropharmacolite, and pink köttigite.

It forms as one of the earliest alteration products of tennantite, chalcopyrite or possibly bornite, under conditions of strongly acidic solutions and rather mobile ions $[AsO_3OH]^{2-}$. It is probable that the rate of crystallisation and the appearance of "pseudo-lindackerite" (lindackerite) depend on pH of the environment. Under sufficiently acidic conditions, crystallisation of "pseudo-lindackerite" (lindackerite) without lavendulan and directly on grains of primary minerals took place.

EDX, WDX		major elements: Cu, As, Ca	minor elements: (Mg)
References		25, 155	

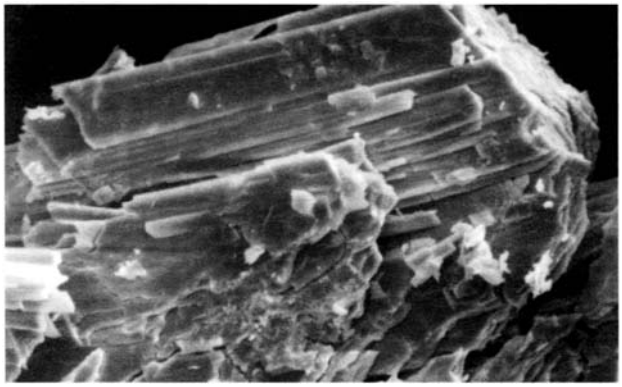
X-ray powder diffraction pattern of "hydronium uranospinite" from Jáchymov.

I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
100	9.647	13	5.646	25	3.574	3	2.859	8	2.1788
66	9.102	6	5.052	5	3.216	8	2.809	6	2.0660
25	8.710	27	4.610	11	3.138	5	2.521	5	2.0280
5	7.905	10	3.950	6	3.006	4	2.4506	5	1.9999
11	7.054	25	3.842	4	2.955	11	2.2727	3	1.7912
3	6.264	6	3.716						

X-ray powder diffraction pattern of "pseudo-lindackerite" from Jáchymov.

I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
3	11.893	5	4.308	11	2.923	1	2.4332	4	1.8718
100	10.667	1	4.039	1	2.850	2	2.3845	1	1.8431
7	7.933	12	3.971	1	2.838	3	2.3387	1	1.8131
2	6.570	4	3.800	1	2.810	2	2.3181	1	1.8063
5	6.193	3	3.699	<1	2.792	2	2.2823	1	1.7741
1	5.842	12	3.649	3	2.758	1	2.2643	<1	1.7598
10	5.342	18	3.560	10	2.736	2	2.2325	1	1.7438
7	5.146	1	3.488	1	2.681	1	2.1559	2	1.7094
1	4.957	2	3.438	3	2.669	4	2.1359	2	1.6568
1	4.780	10	3.286	3	2.648	2	2.0934	2	1.6320
1	4.565	13	3.174	7	2.600	1	2.0192	1	1.6023
1	4.512	2	3.134	3	2.576	4	1.9751	3	1.5886
2	4.484	8	3.097	3	2.564	2	1.9455	1	1.5824
1	4.419	2	3.025	9	2.534	1	1.9320	1	1.5612
1	4.374	3	2.962	6	2.4790	2	1.9004	1	1.5351

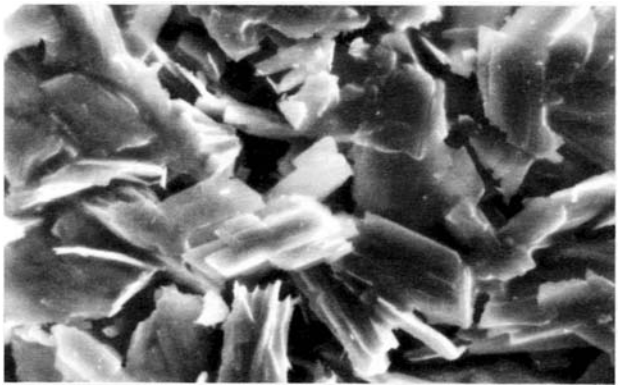
"Pseudo-lindackerite" is documented in Jáchymov in the Geister and Geschieber veins at the Daniel level.



Crystal of "pseudo-lindackerite". Magnification 700

The phase: Cu-AsO_4-H_2O (1)

It occurs as light grey-blue aggregates composed of fine short needles. Radiating aggregates are rare. There is a colour variation with interior of the aggregates being bluish white and surface of a darker colour. The phase Cu-AsO_4-H_2O(1) forms also soft, fine-grained aggregates with a pearly lustre, composed of very fine crystals. The aggregates are greyish white to blue-white.



Imperfectly developed orthorhombic crystals of the phase Cu-AsO_4-H_2O (1). Magnification 1000

They are deposited on vein quartz with chalcopyrite and tennantite. The phase associates with geminite, lindackerite, "pseudo-lindackerite", lavendulan, chalcanthite, erythrite and the phase Cu-AsO_4-H_2O(2).

The specimen was collected in the Geister vein, Rovnost I shaft. Specimen numbers: 82J, 86J.

EDX, WDX		major elements: Cu, As	minor elements: Co, Ni
References		25, 155	

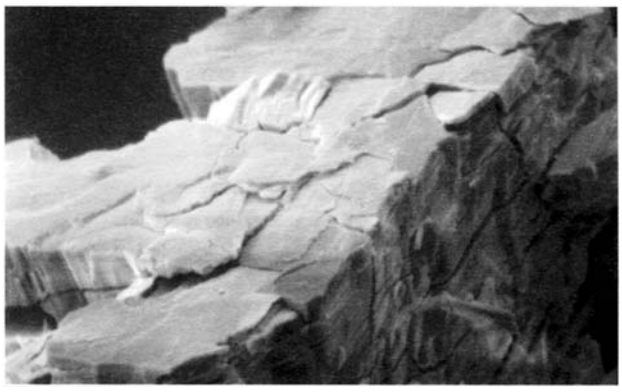
The phase: Cu-AsO_4-H_2O (2)

This phase occurs as brittle aggregates up to 2 mm long, composed of very thin, highly lustrous crystals. It has one set of perfect cleavage and greyish green-blue colour.

The aggregates of Cu-AsO_4-H_2O(2) are deposited on vein quartz with chalcopyrite and tennantite. They occur with geminite, "pseudo-lindackerite", lavendulan, chalcanthite, erythrite and the phase Cu-AsO_4-H_2O(1).

The specimen number 85J carrying this phase was collected in the Geister vein, Rovnost I shaft.

EDX, WDX		major elements: Cu, As	minor elements:
References		25, 155	



Fractured aggregate of the phase Cu-AsO_4-H_2O(2). Magnification 400

X-ray powder diffraction pattern of Cu-AsO_4-H_2O (1) from Jáchymov.

I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	D_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
3	11.597	3	3.921	4	2.975	4	2.3530	1	1.8130
10	9.971	4	3.843	8	2.937	2	2.3048	2	1.7837
100	9.068	3	3.728	1	2.883	1	2.2302	2	1.7460
13	7.784	12	3.529	1	2.837	3	2.2066	2	1.7066
<1	5.698	4	3.365	6	2.760	2	2.1533	4	1.6813
4	4.802	5	3.318	3	2.726	1	2.0699	1	1.6335
2	4.728	4	3.246	2	2.614	2	2.0407	1	1.5363
6	4.388	4	3.081	1	2.555	2	1.9813	1	1.5137
1	4.192	3	3.035	1	2.519	1	1.9545	1	1.5017
1	4.015	4	2.975	1	2.4902	1	1.8836	1	1.4908

X-ray powder diffraction pattern of Cu-AsO_4-H_2O (2) from Jáchymov.

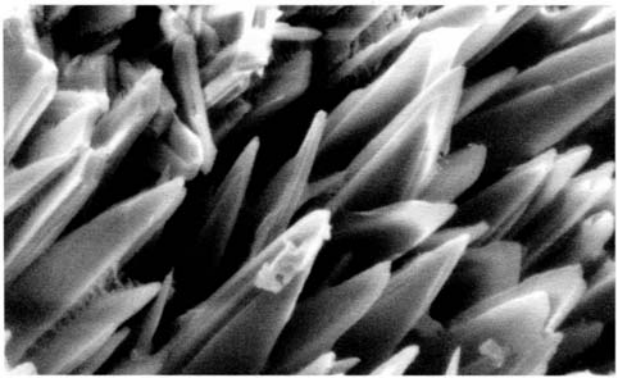
I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
40	10.474	18	3.985	7	2.894	2	2.1420	8	1.7586
100	10.110	8	3.925	8	2.860	1	2.1357	1	1.7267
26	7.940	8	3.907	9	2.842	3	2.1273	3	1.7059
54	7.798	4	3.838	3	2.788	2	2.0828	2	1.6963
3	6.993	9	3.792	6	2.739	3	2.0673	3	1.6786
1	6.454	14	3.651	5	2.689	3	2.0561	2	1.6478
1	6.267	20	3.633	27	2.665	5	2.0419	3	1.6080
16	6.076	5	3.579	6	2.640	9	2.0301	5	1.5953
3	5.820	7	3.494	16	2.609	13	2.0237	3	1.5819
3	5.723	36	3.388	3	2.566	5	2.0028	5	1.5562
2	5.478	24	3.377	7	2.541	4	1.9824	3	1.5532
3	5.215	5	3.313	14	2.534	5	1.9524	5	1.5461
4	5.160	13	3.249	6	2.523	7	1.9458	2	1.5379
30	5.126	29	3.233	3	2.504	1	1.9227	6	1.5279
21	5.073	5	3.188	12	2.4848	8	1.9189	1	1.5185
5	4.957	5	3.162	11	2.4640	5	1.8972	2	1.4851
4	4.748	16	3.136	10	2.4179	3	1.8712	7	1.4744
5	4.470	18	3.106	6	2.3777	3	1.8595	2	1.4704
9	4.408	22	3.047	2	2.3334	9	1.8430	2	1.4396
5	4.339	17	3.040	4	2.2959	3	1.7968	3	1.4205
2	4.270	3	3.004	7	2.2628	2	1.7857	4	1.3932
12	4.162	4	2.965	3	2.2205	8	1.7794	1	1.3837
8	4.007	11	2.913	11	2.2062	9	1.7689	4	1.3785

X-ray powder diffraction pattern of Cu-AsO_4-H_2O (3) from Jáchymov.

I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
3	15.711	2	4.749	4	3.451	1	2.837	1	2.1460
100	11.961	3	4.629	1	3.340	1	2.743	1	2.0916
2	10.882	2	4.533	2	3.322	1	2.697	1	2.0267
1	9.064	<1	4.437	3	3.290	1	2.680	1	2.0099
4	6.994	1	4.263	2	3.236	2	2.605	1	1.9391
1	6.877	1	4.080	1	3.171	1	2.569	<1	1.8971
2	6.179	1	4.019	3	3.140	1	2.544	<1	1.7779
7	5.994	<1	3.928	2	3.081	4	2.4086	1	1.5888
3	5.810	1	3.856	2	3.013	4	2.3992	<1	1.5210
<1	5.181	1	3.818	4	2.970	1	2.3198	<1	1.4512
1	5.078	2	3.726	1	2.913	1	2.3091	<1	1.4229
1	4.965	3	3.597	2	2.895	1	2.2486	1	1.3569
1	4.813	1	3.508	1	2.864	1	2.2175		

The phase: Cu-AsO_4-H_2O (3)

The phase occurs as individual radiating aggregates up to 1 mm in diameter. The non-lustrous, light green-blue aggregates are composed of very fine elongated lustrous crystals.



Radiating aggregates of crystals of the phase Cu-AsO_4-H_2O(3). Magnification 1000

The aggregates crystallised directly on corroded grains of primary sulphides (tennantite, chalcopyrite) or deposited on lavendulan. On its turn, Cu-AsO_4-H_2O(3) is overgrown by a lighter and more lustrous geminite in somewhat larger crystals.

EDX, WDX		major elements: Cu, As	minor elements:
References		25, 155	

The phase Cu-AsO_4-H_2O(3) occurs in paragenesis with lavendulan, geminite, lindackerite and "pseudo-lindackerite".

The specimen studied (number S42a) was collected in the Geschieber vein, at the Daniel level.

The phase: $U^{4+}(HAsO_4)_2$. 4 H_2O

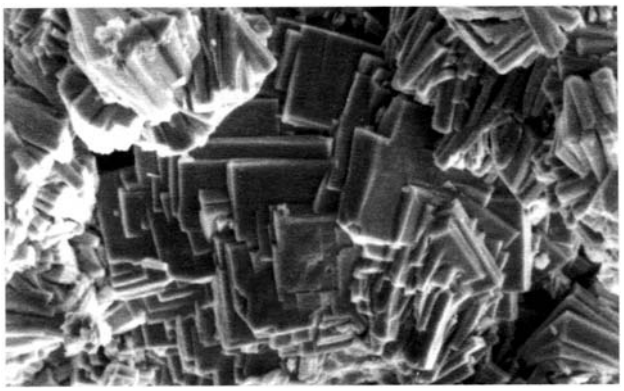
It forms grey-green to dark green crystalline crusts with total surface of several cm^2. The crystals are small, up to 0.1 mm long, platy, with a shape suggesting tetragonal symmetry. It rarely associates with zeunerite. The specimens studied are from the Svornost shaft.

The phase $U(HAsO_4)_2$. 4 H_2O does not fluoresce in UV light. Specimen number: J-406.

X-ray powder diffraction pattern corresponds with the phase $U(HAsO_4)_2$. 4 H_2O listed in the ICDD PDF2 database under number 38-0644.

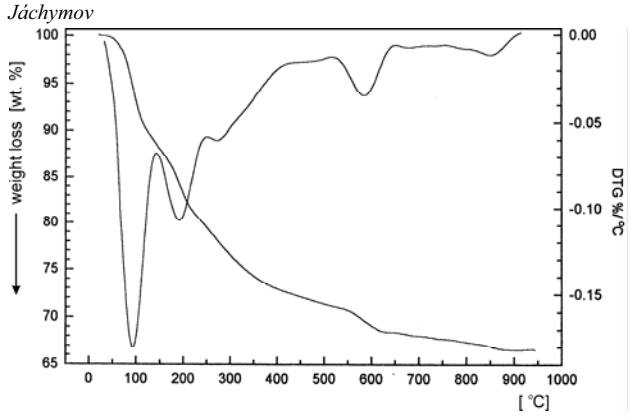
IR [cm^{-1}]		Drift: 408,431,577,667,761,840,931,1233, 1431,1659,2418,3219,3405,3698	
		KBr: 425,559,653,758,816,830,853,869, 936,1004,1035,1076,1236,1402,1652, 3392,3457	
Therm. anal. [°C, wt. %]		20-145 11.8 (partial loss of H_2O), 145-245 8.2 (partial loss of H_2O)	
EDX, WDX		major elements: U, As	minor elements:
References		1, 252	

Tabular crystals of the phase $U(HAsO_4)_2$. 4 H_2O. Magnification 250

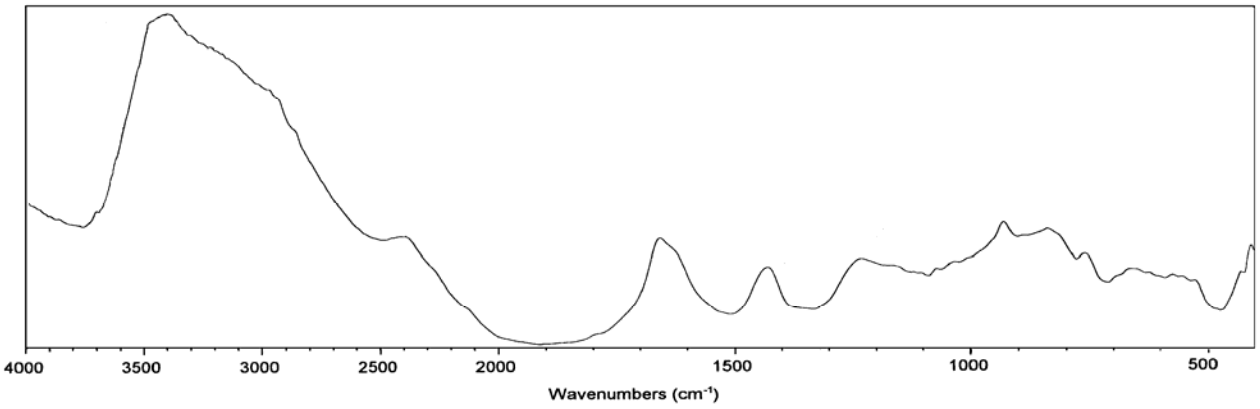


Aggregate of rectangular tabular crystals of the phase $U(HAsO_4)_2$. $4H_2O$. Magnification 500

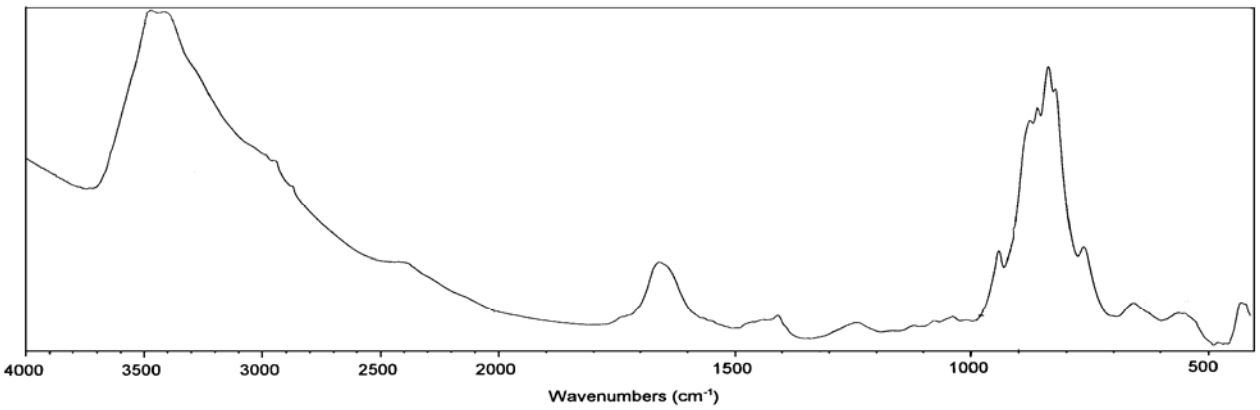
Thermogravimetric (TG, DTG) curves of $U(HAsO4)_2$.4 H_2O from Jáchymov



Infrared absorption spectrum (drift) of $U(HAsO_4)_2$. 4 H_2O from Jáchymov



Infrared absorption spectrum (KBr tablet) of $U(HAsO_4)_2$. 4 H_2O from Jáchymov



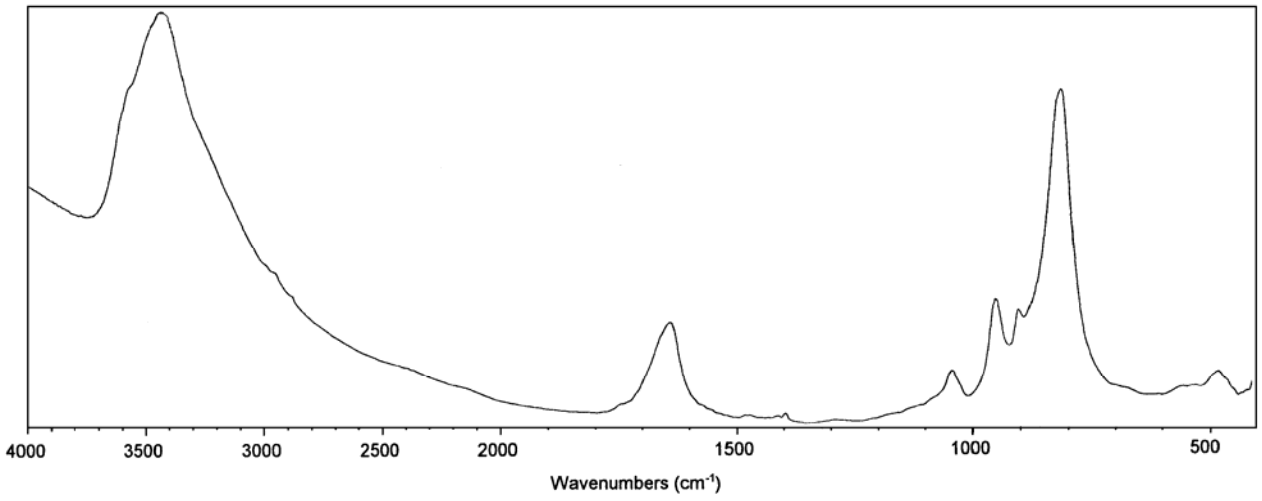
X-ray powder diffraction pattern of $U(HAsO_4)_2 . 4 H_2O$ from Jáchymov.

I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
8	9.085	44	3.400	2	2.1344	10	1.6176	2	1.2422
28	8.711	7	3.342	2	2.1103	2	1.6023	1	1.2299
100	8.228	9	3.293	2	2.0840	3	1.5893	3	1.2247
1	7.169	1	3.225	18	2.0556	4	1.5762	4	1.1829
19	7.027	2	3.197	5	2.0361	3	1.5658	2	1.1716
2	6.397	4	3.034	7	2.0044	3	1.5500	2	1.1579
2	5.600	34	2.933	7	1.9902	4	1.5244	1	1.1484
10	5.501	2	2.823	2	1.9515	10	1.4935	1	1.1385
1	5.216	5	2.769	10	1.9471	2	1.4693	3	1.1335
1	5.069	11	2.748	7	1.9253	1	1.4519	1	1.1180
1	5.025	2	2.689	1	1.8900	4	1.4392	3	1.1066
1	4.965	2	2.659	7	1.8732	2	1.4223	1	1.0942
4	4.866	8	2.608	7	1.8335	5	1.4117	<1	1.0869
2	4.593	6	2.592	1	1.8177	2	1.3968	<1	1.0763
12	4.570	21	2.556	3	1.8010	7	1.3735	3	1.0459
12	4.488	2	2.512	4	1.7894	3	1.3681	2	1.0384
6	4.356	2	2.4556	12	1.7805	3	1.3512	2	1.0287
11	4.110	4	2.3892	7	1.7410	1	1.3361	1	1.0200
27	3.939	8	2.3433	1	1.7158	2	1.3304	1	1.0103
2	3.884	8	2.3198	3	1.6947	4	1.2956	7	0.9911
3	3.831	3	2.2831	5	1.6864	2	1.2785	9	0.9788
9	3.714	21	2.2494	1	1.6610	5	1.2711	3	0.9619
4	3.581	4	2.1779	12	1.6459	2	1.2593	5	0.9492
1	3.553	8	2.1545	3	1.6372				

X-ray powder diffraction pattern of $Ni(UO_2)_2(AsO_4)_2 . 6\text{-}8 H_2O$ from Jáchymov.

I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*	I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*	I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*
100	8.548	8.568	0	0	2	1	3.017	3.007	1	2	2	17	2.1396	2.1421	0	0	8
4	5.070	5.078	1	1	0	2	2.850	2.856	0	0	6	2	2.0533	2.0527	1	0	8
33	4.279	4.284	0	0	4	3	2.810	2.799	1	2	3	1	1.9596	1.9469	1	2	7
5	3.581	3.591	2	0	0	1	2.534	2.539	2	2	0	2	1.8959	1.8931	1	3	5
6	3.424	? 3.427	*0*	*0*	*5*	1	2.509	2.512	2	2	1	1	1.8107	1.8061	2	3	4
3	3.204	3.212	1	2	0	2	2.3722	2.3707	0	3	1	2	1.7528	1.7571	4	0	2
												5	1.7124	1.7127	4	0	3

Infrared absorption spectrum (KBr tablet) of $Ni(UO_2)_2(AsO_4)_2 . 6\text{-}8 H_2O$ from Jáchymov



The phase: $Ni(UO_2)_2(AsO_4)_2 . 6\text{-}8 H_2O$

$Ni(UO_2)_2(AsO_4)_2 . 6\text{-}8 H_2O$ (sample: R13) occurs in light green to yellow-green tabular crystals grown in fractures of vein material.

This phase is sometimes accompanied by zeunerite-metazeunerite. It does not fluoresce in ultra-violet light.

The X-ray powder diffraction pattern is very close to patterns of tetragonal phases: metakirchheimerite [329] $Co(UO_2)_2(AsO_4)_2 . 8 H_2O$ and $Ni(UO_2)_2 (AsO_4)_2 . 8H_2O$ (ICDD 12-586 [275]). The diffractions observed were indexed with the space group P4/nmm. However, powder diffraction data generated from the structural data (modified for Ni) for meta-autunite [326], meta-zeunerite [327], metatorbernite [328] are not identical with the diffraction pattern of the phase $Ni(UO_2)_2 (AsO_4)_2 . 6\text{-}8 H_2O$ from Jáchymov.

X-ray powder diffraction pattern of $PbO-UO_3-H_2O$ from Jáchymov.

I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
2	16.993	2	4.174	23	2.901	5	2.1720	8	1.8121
6	16.155	7	4.069	6	2.821	8	2.1068	13	1.8039
5	10.280	13	3.967	16	2.763	2	2.0899	3	1.7537
9	8.825	27	3.924	11	2.704	7	2.0668	11	1.7221
40	7.907	38	3.895	20	2.619	10	2.0318	4	1.6735
100	7.630	10	3.813	6	2.575	10	2.0205	4	1.6424
78	7.071	40	3.691	3	2.547	14	1.9790	4	1.6082
8	6.354	44	3.542	3	2.509	9	1.9626	4	1.5728
12	5.934	14	3.479	5	2.4897	4	1.9509	5	1.5520
5	5.705	21	3.355	6	2.4301	6	1.9315	4	1.5307
35	5.641	11	3.277	2	2.3927	3	1.9208	7	1.5105
12	5.005	83	3.216	12	2.3551	18	1.8934	4	1.3873
4	4.953	21	3.170	4	2.2893	7	1.8799	3	1.3078
6	4.457	4	3.099	6	2.2557	13	1.8563	3	1.2705
1	4.340	9	3.039	4	2.2254	7	1.8193		
7	4.258	11	3.004	4	2.1995				

X-ray powder diffraction pattern of UO_3 - H_2O (1) from Jáchymov.

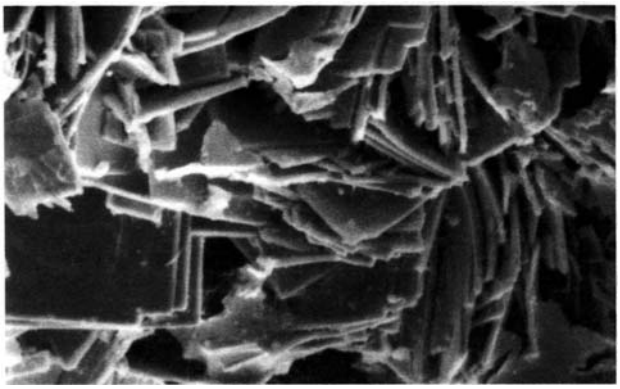
I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
34	10.286 *	6	6.513	1	3.690	5	3.223	2	2.4502
34	9.743	13	5.772	11	3.629	10	3.185	3	2.4108
8	9.234	3	5.508	15	3.579 *	5	3.112	5	2.2054
10	8.727	3	5.197 *	31	3.547	8	2.957	1	2.1791
100	7.836	7	5.059	7	3.448	5	2.811	3	2.0459
15	7.491	21	4.013	3	3.375 *	9	2.723	4	2.0309
74	7.257	5	3.928	9	3.349	4	2.532	3	1.9890
6	6.514	10	3.789	26	3.263				

"" – diffractions of zeunerite*

X-ray powder diffraction pattern of UO_3 - H_2O (2) from Jáchymov.

I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
44	10.641	22	6.034	13	4.030	94	3.250	35	2.542
20	8.476	14	5.764	33	3.763	43	3.198	22	2.4597
73	7.944	7	5.261	64	3.623	27	2.947	22	2.2687
67	7.588	25	5.110	47	3.582	20	2.779	26	2.0461
100	7.363	29	5.024	28	3.538	18	2.592	23	1.9893
22	6.866	21	4.559	31	3.400				

Lattice par. [Å]	a =7.1811(4)		c = 17.14(2)
	V=883.7(11) tetragonal, S.G. P42/m or P4/nmm, Z=2		
EDX, WDX	major elements: U, As, Ni	minor elements:	
IR [cm^{-1}]	477,811,897,946,1035,1628,3417		
References	275, 326, 327, 328		



Aggregate of tetragonal tabular crystals of the phase $Ni(UO_2)_2(AsO_4)_2$. $6\text{-}8H_2O$. Magnification 500

The phase: $PbO-UO_3-H_2O$

The phase $PbO-UO_3-H_2O$ was identified on a single specimen. It forms yellow-brown to orange very thin glassy coatings, several mm^2 in size. The coatings are deposited on strongly silicified vein material next to partly weathered uraninite. The phase $PbO-UO_3-H_2O$ is associated with radiating aggregates of uranophane and clinochlore. The specimen No. 106 was collected on dump of the Rovnost I mine.

EDX, WDX		major elements: U, Pb	minor elements: (P, Si, Ca)

The phase: UO_3 - H_2O (1)

The phase $UO_3-H_2O(1)$ was identified in a single specimen. It forms up to 0.5 mm thick orange-brown coatings of glassy appearance, with indistinct fibrous structure.

EDX, WDX		major elements: U	Minor elements: Pb

X-ray powder diffraction pattern of "pseudo-zippeite (Mg)" from Jáchymov.

I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
4	12.724	1	3.670	7	2.679	7	2.0894	3	1.7334
100	9.574	6	3.640	1	2.650	2	2.0488	15	1.7198
31	8.534	10	3.561	13	2.586	8	2.0299	6	1.7111
1	7.576	11	3.484	4	2.558	6	2.0088	13	1.6853
1	6.988	81	3.438	3	2.4926	10	1.9650	7	1.6428
1	6.867	3	3.361	4	2.4787	7	1.9248	5	1.5906
20	6.382	23	3.201	12	2.4527	1	1.9031	1	1.5706
13	5.992	2	3.123	5	2.4020	1	1.8913	3	1.5355
7	5.167	43	3.068	4	2.3189	3	1.8693	2	1.5140
56	4.797	3	3.017	6	2.2922	2	1.8369	3	1.5053
2	4.421	3	2.928	3	2.2463	6	1.8214	2	1.4837
33	4.274	44	2.852	19	2.2119	4	1.7860	3	1.4751
29	4.176	4	2.787	19	2.1557	1	1.7718	3	1.4657
20	3.903	29	2.734	8	2.1406	18	1.7479	2	1.4539
11	3.749	9	2.709	25	2.1261	22	1.7395	2	1.4470

The phase UO_3-H_2O(1) is a direct product of weathering of uraninite. It is associated with brown-yellow richetite, green aggregates of antlerite, zeunerite, langite, and light green to light yellow aggregates of tabular metazeunerite and nováčekite (sample No. J-359).

X-ray powder diffraction data correspond to unnamed mineral from El Sherana mine, South Alligator district, Northern Territory, Australia (Threadgold in [275] – ICDD card 15-569).

The phase: UO_3 - H_2O (2)

The material forms local pseudomorphs after uraninite by replacing it along fractures. It is compact, brittle and has an olive yellow colour. It does not fluoresce in UV light. Fracture is uneven with a greasy lustre. The phase UO_3-H_2O (2) was identified in a mixture with compreignacite (sample No. VS-19256b).

EDX, WDX		major elements: U	minor elements:
References		21	

"Pseudo-zippeite(Mg)" (Mg,Fe, K_2)O-UO_3-SO_3-H_2O

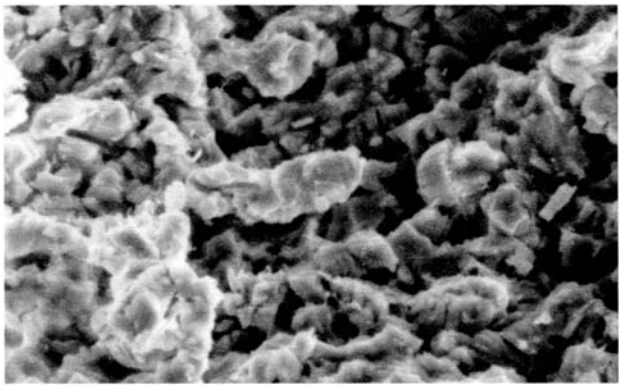
The phase "pseudo-zippeite (Mg)" (sample: 71J) occurs in powdery coating or as earthy aggregates, which are strong yellow, usually in mixture with zippeite, sodium-zippeite, uranopilite, jáchymovite, and other phases. Aggregates of "pseudo-zippeite (Mg)" show variety of habits, including earthy, granular/crystalline, and soft or hardened intense yellow to orange to red brownish yellow. It is this variability in appearance, which decisively contributed to ignorance of additional associated phases, which can not be recognised and identified without a detailed study. Jáchymovite, "pseudo-zippeite (Mg)" and zippeite can serve as example of the latter minerals.

EDX, WDX		major elements: U, S	minor elements: (Na, Ca)
References		24, 35, 132, 152, 191, 205, 252, 260	

The phase "pseudo-zippeite (Mg)" was described as associated with zippeite, gypsum, uranopilite, sodium-zippeite, johannite, exceptionally jáchymovite, sklodowskite and metaschoepite.

The weak fluorescence in ultra-violet light is dark olive brown.

See also other minerals of the zippeite group (sodium-zippeite, zippeite, nickel-zippeite, magnesium-zippeite, "ferro-zippeite").



Detail of earthy, poorly defined crystals of the phase "pseudo-zippeite (Mg)". Magnification 800

"Ferro-zippeite" $[(Fe,Mg)(UO_2)_2(SO_4)(OH)_4]_2 \cdot 3\ H_2O$

"Ferro-zippeite" (sample U10) often occurs in powdery coating or as earthy aggregates, in mixture with other uranium sulphates, which include several types of zippeite (Na, K, Mg, Ni, Mn) with various cations, "pseudo-zippeite (Mg)", uranopilite, jáchymovite, and other phases. "Ferro-zippeite" aggregates show variety of habits, including earthy, granular/crystalline, and soft or hardened intense yellow to orange to red brownish yellow.

The specimens were collected in the Evangelista vein.

Occasionally, it forms isolated crystals and their radiating aggregates, probably favoured by lower-concentration solutions and a moderate pH gradient.

X-ray powder diffraction pattern of "ferro-zippeite" from Jáchymov.

I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*	I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*	I_{rel}	d_{obs}
* 33	9.558					4	3.338					4	2.2865
6	9.111					4	3.307					16	2.2379
* 24	8.638	8.613	0	0	2	* 4	3.186					4	2.1380
8	7.686					17	3.117	3.121	2	2	2	2	2.0762
100	7.189	7.197	0	2	0	17	3.117	3.120	2	2	-4	5	2.0500
* 1	6.373					* 5	3.061					6	1.9616
* 1	6.000					* 20	2.867	2.871	0	0	6	3	1.9533
10	5.516	5.523	0	2	2	3	2.745					3	1.8321
* 13	4.770					3	2.697	2.699	2	0	4	5	1.7865
13	4.307	4.306	0	0	4	3	2.671	2.667	0	2	6	7	1.7475
4	4.216	4.209	2	0	0	15	2.660	2.658	1	5	1	3	1.7296
* 3	4.158					1	2.528	2.527	2	2	4	2	1.7186
3	3.943	3.944	1	3	1	6	2.4951	2.4953	2	4	2	6	1.6985
* 3	3.929					6	2.4951	2.4949	2	4	-4	2	1.6792
5	3.691	3.695	0	2	4	5	2.4867					1	1.5842
40	3.577	3.586	1	3	-3	9	2.3818	2.3990	0	6	0	3	1.5702
23	3.466	3.463	2	0	2	9	2.3818					2	1.5539
23	3.466	3.462	2	0	-4	2	2.2963	2.3110	0	6	2	2	1.5485
* 7	3.433					2	2.2963					2	1.5421

** - diffractions corresponding to "pseudo-zippeite (Mg)"*

X-ray powder diffraction pattern of $PbO-UO_3-SO_3-H_2O$ from Jáchymov.

I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
7	8.873	2	4.730	20	3.255	4	2.723	3	1.9693
44	7.903	5	4.597	7	3.215	5	2.4946	2	1.9548
50	7.406	7	4.437	5	3.157	3	2.4707	6	1.9300
100	7.162	4	4.263	11	3.132	5	2.3990	3	1.8540
3	6.832	2	4.209	2	3.078	5	2.3740	2	1.7989
10	6.512	10	4.097	4	3.007	3	2.2796	5	1.7816
4	6.420	21	3.954	1	2.947	4	2.1711	4	1.7471
5	6.069	22	3.708	5	2.916	2	2.0880	3	1.6788
9	6.010	49	3.577	2	2.882	3	2.0668	2	1.6273
2	5.829	10	3.483	6	2.811	5	2.0275	2	1.5844
3	5.280	3	3.337	9	2.772	8	2.0053		

"Ferro-zippeite" was described as associated with gypsum, uranopilite, zippeite, sodium-zippeite, nickel-zippeite, magnesium-zippeite, johannite, "pseudo-zippeite (Mg)", exceptionally jáchymovite, sklodowskite, metaschoepite.

In present study, mixtures of "pseudo-zippeite (Mg)" always with zippeites (all types) were regularly observed.

On a basis of a structure of a synthetic zinc-zippeite [152] and a chemical analogy of isostructural zippeites (Ni, Mg, Co, Zn, Mn, Cd) [132], it is possible to proposed a chemical formula for magnesium-zippeite as follows:

$$[Fe(UO_2)_2(SO_4)(OH)_4]_2 \cdot 3\ H_2O$$

See also other minerals of the zippeite group (sodium-zippeite, zippeite, nickel-zippeite, mahnesium-zippeite, "pseudo-zippeite (Mg)").

Lattice par. [Å, °]		a = 8.681(7)	b= 14.39(1)	c =17.76(1)
			β=104.13(1)	
EDX, WDX		major elements: U, S, Fe		minor elements: Mg, K
References		132, 152, 161, 165, 170, 252, 260		

Phase $PbO-UO_3-SO_3-H_2O$

The phase $PbO-UO_3-SO_3-H_2O$ (sample No.: 25Ja) was found on a single specimen.

It occurs in powdery coating or as earthy aggregates, which are strong orange.

The phase $PbO-UO_3-SO_3-H_2O$ is associated with yellow crystalline dewindtite.

The specimen was collected in the Rovnost I. shaft.

EDX, WDX		major elements: U, Pb, S	minor elements: K
References		24, 35, 132, 152, 191, 205, 252, 260	

"Phosphate-walpurgite" $Bi_4(UO_2)(PO_4)_2O_4 \cdot 2H_2O$

The phase occurs as greasy lustrous "eyes" up to 1 cm in diameter, as a rule rimmed by coarsely crystallised torbernite, in a strongly cavernous vein. It is waxy yellow and has a conchoidal fracture. It also rarely occurs as yellow prismatic crystals up to 2 mm long, which are glassy or show a waxy lustre. We also studied specimens carrying "phosphate-walpurgite" as compact light brown olive crusts associated with light green torbernite, coating silicified gneiss.

It occurs in paragenesis with torbernite, grey-yellow, powdery preisingerite and petitjeanite on the Geister vein.

X-ray powder diffraction patterns of two samples of "phosphate-walpurgite" from Jáchymov.

JG-35519						J-87						JG-35519						J-87					
I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*	I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*	I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*	I_{rel}	d_{obs}	d_{calc}	*h*	*k*	*l*
100	10.199	10.198	0	1	0	100	10.404	10.395	0	1	0	39	3.052	3.053	1	3	-1						
65	6.665	6.660	1	0	0	36	6.713	6.712	1	0	0							10	2.885	2.874	-2	2	0
70	5.692	5.690	-1	1	0							31	2.734	2.742	1	1	-2	11	2.748	2.741	1	1	-2
30	5.472	5.470	1	1	0							5	2.585					9	2.594	2.599	0	4	0
14	5.079	5.100	0	2	0	24	5.205	5.197	0	2	0							8	2.526	2.523	0	-4	1
						55	5.011	5.043	0	0	1	18	2.515	2.513	0	0	2						
69	4.957	4.959	-1	0	1	25	4.959	4.958	-1	0	1							19	2.505	2.506	2	1	-2
7	4.164	4.136	-1	2	0													7	2.4635	2.4621	-2	3	0
42	4.023	4.008	0	2	-1													21	2.4349	2.4319	2	-1	1
13	3.965	3.967	1	2	0													13	2.1911	2.1940	2	3	-2
						26	3.469	3.465	0	3	0	24	2.4169	2.4163	-1	4	0						
17	3.450	3.449	1	-1	1	8	3.440	3.474	1	-1	1	25	2.1872	2.1855	2	3	-2						
14	3.396	3.394	-2	0	1													3	2.1650	2.1630	2	4	-1
50	3.266	3.264	0	2	1							<1	2.0680	2.0684	-3	2	0						
57	3.127	3.125	0	3	-1							20	2.0680	2.0680	-2	4	0						
32	3.104	3.105	1	-2	1	3	3.127	3.133	1	-2	1	11	1.9265	1.9273	1	5	0						

The X-ray powder diffraction patterns of "phosphate-walpurgite" tend rather regularly to broadened diffraction profiles and to absence of some diffraction. This is probably caused by poor stability of the $Bi_4(UO_2)(PO_4)_2O_4 \cdot 2H_2O$ crystal structure, which is probably identical to that of $Bi_4(UO_2)(AsO_4)_2O_4 \cdot 2H_2O$ (walpurgite). Unit cell parameters and diffraction indices for the uranyl-phosphate phase were calculated on the basis of similarity to walpurgite.

Lattice par. [Å, °]	1	a = 7.141(6)	b=10.421(8)	c = 5.497(3)
		α=101.57 (1)	β=111.01(1)	γ=88.137(8)
	2	a = 7.18(2)	b=10.61(3)	c = 5.50(1)
		α=101.33(3)	β=110.59(4)	γ=88.22(3)
EDX, WDX		major elements: Bi, U, P		minor elements: Fe, Cu, V, Zn, As
References		122		

1 - J-87, greasy lustrous waxy yellow "eyes"
2 - JG-35519, light brown olive compact crust

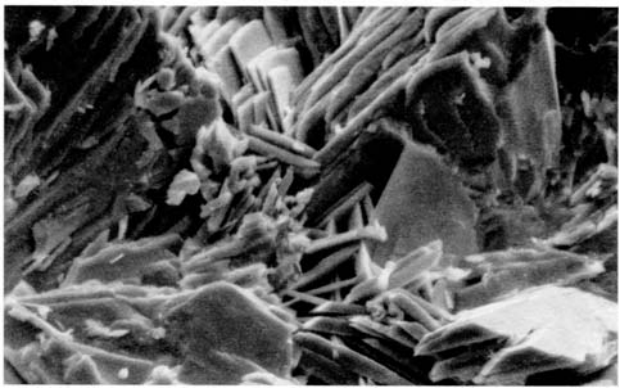
"Mg-villyaellenite"
$(Mg,Ca,Zn)_5(AsO_4)_2[AsO_3(OH)]_2 \cdot 4\ H_2O$

"Mg-villyaellenite" occurs in hard small spheres, less than 1 mm in diameter, in part clustered in grape-like aggregates. Some spheres are hollow, others are composed of radiating acicular crystals. The spheres are milky white to vitreous transparent.

Lattice par. [Å, °]	1	a = 18.588(2)	b = 9.4130(9)	c = 9.9762(8)
			β= 96.907(6)	
EDX, WDX		major elements: Ca, As, Mg		minor elements:
References		69, 71, 151, 130		

1 – "Mg-villyaellenite", Jáchymov - Rietveld refinement

"Mg-villyaellenite" is in association with extraordinary large crystals of haidingerite, picropharmacolite and pharmacolite. It was identified in a sample in a collection of Moravian Museum in Brno (sample No. BM-A1840a).



Aggregate of tabular crystals of "Mg-villyaellenite". Magnification 500

"Kalium-schröckingerite"

The phase forms powdery coating or compact earthy aggregates on the surface of specimen collected in 1915 (sample No.: PF-6470). The surface of the coating tends to a glassy appearance and carries indistinct vicinal crystal faces. The phase is yellow with a shade of ochre. It fluoresces an intense light green, rather similar as schröckingerite. It is not accompanied by any other secondary mineral.

X-ray powder diffraction pattern of "kalium-schröckingerite" is similar to pattern of schröckingerite (see table below).

EDX, WDX		major elements: U, S, Ca, K	minor elements: Mg, (Si)

X-ray powder diffraction pattern of Mg- villyaellenite calculated from Rietveld refinement. Calculated intensities are compared to observed intensities of Mg- villyaellenite from Jáchymov.

I_{obs}	I_{calc}	*h*	*k*	*l*	d_{calc}	I_{obs}	I_{calc}	*h*	*k*	*l*	d_{calc}	I_{obs}	I_{calc}	*h*	*k*	*l*	d_{calc}
73	50	2	0	0	9.226	2	3	6	2	-2	2.3846	14	14	3	3	4	1.8051
38	37	1	1	0	8.385	2	2	3	3	2	2.3790	14	16	5	3	-4	1.7909
8	11	1	1	-1	6.579	17	20	7	1	-2	2.3733	7	8	3	1	5	1.7893
3	12	1	1	1	6.234	3	3	5	3	-1	2.3662	2	2	4	2	-5	1.7659
2	1	0	0	2	4.952	2	2	0	4	0	2.3532	2	2	2	2	5	1.7543
20	22	3	1	-1	4.769	3	4	1	1	4	2.3402	6	6	1	5	2	1.7448
25	27	0	2	0	4.707	26	20	8	0	0	2.3066	6	6	4	4	3	1.7274
43	46	4	0	0	4.613	28	24	4	0	-4	2.2999	16	13	9	3	-1	1.7205
42	46	2	0	-2	4.600	7	7	0	4	1	2.2895	3	2	10	2	0	1.7180
52	59	3	1	1	4.391	2	2	1	3	-3	2.2803	3	2	9	3	0	1.7164
2	2	1	1	-2	4.370	2	2	2	4	0	2.2803	7	7	3	5	-2	1.7113
9	10	0	2	1	4.251	6	8	5	1	3	2.2576	5	4	6	4	2	1.7078
5	6	2	2	0	4.193	5	7	2	4	-1	2.2367	10	10	0	4	4	1.7058
14	16	1	1	2	4.165	5	6	1	3	3	2.2349	3	3	2	4	-4	1.7027
17	19	2	0	2	4.160	13	14	2	4	1	2.2078	12	12	10	2	-2	1.6824
24	25	2	2	-1	3.939	2	1	6	2	2	2.1956	4	4	6	4	-3	1.6799
20	24	2	2	1	3.787	2	1	8	0	-2	2.1944	2	2	5	5	0	1.6770
3	4	3	1	-2	3.763	2	2	3	3	-3	2.1931	8	9	9	3	-2	1.6747
2	<1	4	0	-2	3.598	8	7	0	2	4	2.1912	4	4	3	5	2	1.6731
7	5	5	1	0	3.436	2	3	7	1	2	2.1597	6	6	10	2	1	1.6616
24	22	0	2	2	3.411	3	3	3	1	4	2.1485	9	9	2	0	-6	1.6598
16	16	3	1	2	3.402	2	2	6	2	-3	2.1372	2	2	3	3	-5	1.6595
100	100	5	1	-1	3.365	16	18	7	1	-3	2.1354	5	6	7	3	3	1.6555
7	8	4	2	0	3.294	3	4	5	1	-4	2.1248	10	11	1	3	5	1.6530
86	91	2	2	-2	3.290	10	10	4	4	0	2.0963	4	4	6	2	-5	1.6524
37	36	4	2	-1	3.210	3	3	2	4	-2	2.0950	4	4	0	0	6	1.6507
9	8	4	0	2	3.190	7	8	5	3	2	2.0900	2	2	7	3	-4	1.6401
17	18	5	1	1	3.139	3	3	4	0	4	2.0799	2	3	5	5	1	1.6388
2	2	1	1	-3	3.131	11	11	3	3	3	2.0779	8	10	5	1	5	1.6385
61	69	2	2	2	3.117	3	3	4	4	-1	2.0739	3	4	1	5	-3	1.6376
18	15	6	0	0	3.076	5	4	4	2	-4	2.0664	3	4	4	2	5	1.6367
40	48	1	1	3	3.016	6	6	6	0	-4	2.0530	3	4	5	5	-2	1.6154
6	6	1	3	-1	2.970	4	5	2	4	2	2.0482	5	6	1	1	6	1.6031
24	22	3	1	-3	2.916	11	12	7	3	0	2.0183	3	3	8	4	1	1.6028
17	17	4	2	-2	2.859	2	3	7	3	-1	2.0143	4	4	11	1	1	1.5986
13	13	3	3	0	2.795	7	8	5	3	-3	2.0121	3	3	8	0	4	1.5948
11	9	6	0	-2	2.766	9	9	9	1	-1	2.0100	8	11	5	3	-5	1.5872
9	8	3	3	-1	2.729	10	7	8	2	1	1.9849	2	2	6	4	3	1.5777
18	20	0	2	3	2.703	4	4	7	3	1	1.9430	4	5	3	3	5	1.5760
21	19	5	1	2	2.686	3	2	9	1	-2	1.9380	19	21	10	2	2	1.5696
6	6	3	1	3	2.660	5	4	7	3	-2	1.9323	5	6	2	2	-6	1.5653
10	12	3	3	1	2.652	2	2	9	1	1	1.9202	7	8	5	5	2	1.5627
2	2	1	3	-2	2.648	2	2	0	4	3	1.9162	4	4	0	2	6	1.5576
4	4	4	2	2	2.640	3	3	3	1	-5	1.9144	3	3	11	1	-3	1.5524
2	2	1	3	2	2.600	2	2	2	4	-3	1.9028	6	6	0	6	1	1.5495
3	1	6	2	0	2.575	2	3	4	4	2	1.8936	4	4	6	4	-4	1.5470
4	2	6	2	-1	2.555	7	9	6	4	0	1.8689	6	7	2	6	0	1.5466
19	18	7	1	-1	2.530	4	4	5	3	3	1.8683	18	13	12	0	0	1.5377
12	11	2	2	3	2.527	7	6	1	5	-1	1.8444	4	3	6	0	-6	1.5333
23	23	0	0	4	2.4760	5	4	8	2	2	1.8413	4	4	7	5	0	1.5320
7	7	2	0	-4	2.4668	7	6	1	5	1	1.8362	9	9	4	2	-6	1.5293
8	7	4	2	-3	2.4391	5	5	4	4	-3	1.8151	2	2	5	5	-3	1.5293
8	6	6	2	1	2.4328	3	3	9	1	-3	1.8096	6	8	2	4	-5	1.5179
26	27	7	1	1	2.3932	5	5	5	1	-5	1.8058	2	3	8	2	-5	1.5156
32	34	5	3	0	2.3905												

X-ray powder diffraction pattern of "kalium-schröckingerite" from Jáchymov.

I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
18	14.523	52	4.806	8	3.597	7	2.777	4	2.3107
15	8.498	10	4.410	16	3.504	6	2.687	15	2.2587
23	7.657	19	4.297	14	3.244	7	2.4995	4	2.2227
100	7.224	6	4.182	15	3.076	12	2.4449	8	1.7973
15	6.784	7	4.068	8	3.055	9	2.3990	5	1.6195
17	5.448	9	3.815	64	2.879				

X-ray powder diffraction pattern of Zn-AsO_4-H_2O from Jáchymov.

I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}	I_{rel}	d_{obs}
82	11.209	14	6.852	4	4.400	50	3.341	5	2.678
68	9.707	100	6.710	5	4.250	23	3.189	6	2.3825
3	8.928	2	4.989	9	3.734	3	3.032	3	2.2846
1	8.475	3	4.808	4	3.580	8	2.942	2	2.2631
2	7.602	4	4.565	3	3.459	4	2.888	6	2.2413
33	7.081	4	4.449	11	3.360	10	2.802	6	1.5959

The phase: Zn-AsO_4-H_2O

The phase Zn-AsO_4-H_2O forms hard spheres up to 0.5 mm in diameter, showing a radiating fibrous structure. The spheres show zoning consisting of alternation of milky and glassy layers. The spheres are white, with a mat surface and a glassy lustre on fractures. It is deposited directly on wall rock and tends to be covered by amorphous glassy blue-green flakes containing Zn, As, Ca and Mn as the main elements (Mg is absent). The specimens were collected in the Geister vein.

EDX, WDX		major elements: Zn, As	minor elements: Mn

The phase: $Ca_2(UO_2)_2(Si_2O_5)_3 \cdot 10H_2O$

It forms thin coating of about 0.5 cm^2 on a weathered sample. The coating is made of thin tabular crystals with diameter 20-30 μm and thickness about 1-2 μm. Its colour is yellow. The coating is transparent and has vitreous lustre. It fluoresces intensively, colour is greenish yellow. It was find in association with gypsum, rösslerite, liebigite, zellerite, voglite, and unnamed phase Cu-Ca-UO_2-CO_3-H_2O. The sample originates from the vein No. 3.

Lattice par. [Å]		a= 12.075(18)	b =15.406(27)	c =26.043(22)
	1	a = 12.075(3)	b = 15.406(6)	c =26.043(6)
EDX, WDX		major elements: Ca, U, Si		minor elements:
References		275		

1 - Synthetic $Ca_2(UO_2)_2(Si_2O_5)_3 \cdot 10H_2O$ – Moroni et al.in [275] (ICDD card 47-0497).

Acknowledgements

This study was supported by the Grant Agency of the Czech Republic, grants No. 205/93/0900 and No. 205/97/0491.

List of five most intensive reflections for unnamed secondary mineral phases of the Jáchymov ore district.

1	**16.22**	$Mg\text{-}AsO_4\text{-}H_2O$	1	**7.363**	$UO_3 - H_2O$ (2)	4	**3.581**	$Ni(UO_2)_2(AsO_4)_2$. 6-8 H_2O
5	**14.52**	"kalium-schröckingerite"	2	**7.257**	$UO_3 - H_2O$ (1)	3	**3.577**	$PbO\text{-}UO_3\text{-}SO_3\text{-}H_2O$
1	**12.48**	$Fe\text{-}AsO_4\text{-}H_2O$(1)	1	**7.224**	"kalium-schröckingerite"	2	**3.560**	"pseudo-lindackerite"
1	**11.96**	$Cu\text{-}AsO_4\text{-}H_2O$ (3)	4	**7.178**	"pseudo-voglite"	2	**3.558**	$Ca(H_2AsO_4)_2$
1	**11.95**	$Ca\text{-}Mg\text{-}AsO_4\text{-}H_2O$	1	**7.162**	$PbO\text{-}UO_3\text{-}SO_3\text{-}H_2O$	3	**3.551**	$Ca\text{-}Mg\text{-}AsO_4\text{-}H_2O$
2	**11.21**	$Zn\text{-}AsO_4\text{-}H_2O$	2	**7.110**	"pseudo-johannite"	5	**3.547**	$UO_3 - H_2O$ (1)
1	**10.99**	$Ca\text{-}Cu\text{-}(UO_2)\text{-}(CO_3)\text{-}H_2O$	5	**7.081**	$Zn\text{-}AsO_4\text{-}H_2O$	4	**3.542**	$PbO\text{-}UO_3\text{-}H_2O$
1	**10.81**	"pseudo-voglite"	3	**7.071**	$PbO\text{-}UO_3\text{-}H_2O$	3	**3.529**	$Cu\text{-}AsO_4\text{-}H_2O$ (1)
1	**10.67**	"pseudo-lindackerite"	5	**7.027**	$U(HAsO_4)_2$. 4 H_2O	3	**3.457**	$[(MoO_2)_2As_2O_5(H_2O)_2]$. H_2O
3	**10.47**	$Cu\text{-}AsO_4\text{-}H_2O$(2)	3	**6.994**	$Cu\text{-}AsO_4\text{-}H_2O$ (3)	4	**3.451**	$Cu\text{-}AsO_4\text{-}H_2O$ (3)
1	**10.39**	$Ca\text{-}(VO)\text{-}AsO_4$	1	**6.915**	$[(MoO_2)_2As_2O_5(H_2O)_2]$. H_2O	2	**3.438**	"pseudo-zippeite (Mg)"
1	**10.20**	"phosphate-walpurgite"	5	**6.811**	$Fe\text{-}AsO_4\text{-}H_2O$(2)	4	**3.434**	$[(MoO_2)_2As_2O_5(H_2O)_2]$. H_2O
1	**10.11**	$Cu\text{-}AsO_4\text{-}H_2O$(2)	1	**6.710**	$Zn\text{-}AsO_4\text{-}H_2O$	5	**3.424**	$Ni(UO_2)_2(AsO_4)_2$. 6-8 H_2O
4	**9.971**	$Cu\text{-}AsO_4\text{-}H_2O$(1)	4	**6.665**	"phosphate-walpurgite"	5	**3.410**	$Ca_2Cu(UO_2)_2(CO_3)_2O_3$. 3 H_2O
3	**9.743**	$UO_3 - H_2O$ (1)	3	**6.433**	$Ca\text{-}(VO)\text{-}AsO_4$	2	**3.400**	$U(HAsO_4)_2$. 4 H_2O
3	**9.707**	$Zn\text{-}AsO_4\text{-}H_2O$	4	**6.428**	$Ca\text{-}Cu\text{-}(UO_2)\text{-}(CO_3)\text{-}H_2O$	4	**3.388**	$Cu\text{-}AsO_4\text{-}H_2O$ (2)
2	**9.657**	"pseudo-voglite"	2	**6.266**	$Fe\text{-}AsO_4\text{-}H_2O$(1)	1	**3.365**	"Mg- villyaellenite"
1	**9.647**	"hydronium uranospinite"	3	**6.250**	$Ca_2Cu(UO_2)_2(CO_3)_2O_3$. 3 H_2O	4	**3.341**	$Zn\text{-}AsO_4\text{-}H_2O$
1	**9.574**	"pseudo-zippeite (Mg)"	2	**6.046**	$[(MoO_2)_2As_2O_5(H_2O)_2]$. H_2O	5	**3.324**	$[(MoO_2)_2As_2O_5(H_2O)_2]$. H_2O
2	**9.543**	$Ca\text{-}Cu\text{-}(UO_2)\text{-}(CO_3)\text{-}H_2O$	2	**5.994**	$Cu\text{-}AsO_4\text{-}H_2O$ (3)	2	**3.290**	"Mg- villyaellenite"
1	**9.497**	$Fe\text{-}AsO_4\text{-}H_2O$(2)	2	**5.692**	"phosphate-walpurgite"	4	**3.263**	$UO_3 - H_2O$ (1)
2	**9.308**	$Fe\text{-}AsO_4\text{-}H_2O$(2)	4	**5.684**	$Ca_2Cu(UO_2)_2(CO_3)_2O_3$. 3 H_2O	3	**3.262**	$Ca(H_2AsO_4)_2$
3	**9.226**	"Mg- villyaellenite"	3	**5.527**	"pseudo-johannite"	2	**3.250**	$UO_3 - H_2O$ (2)
1	**9.134**	"pseudo-johannite"	5	**5.342**	"pseudo-lindackerite"	4	**3.246**	$Ca\text{-}Mg\text{-}AsO_4\text{-}H_2O$
2	**9.102**	"hydronium uranospinite"	5	**5.126**	$Cu\text{-}AsO_4\text{-}H_2O$ (2)	4	**3.244**	$Mg\text{-}AsO_4\text{-}H_2O$
1	**9.094**	$Ca_2Cu(UO_2)_2(CO_3)_2O_3$. 3 H_2O	3	**4.957**	"phosphate-walpurgite"	5	**3.229**	$Na_4(UO_2)(CO_3)_3$
1	**9.068**	$Cu\text{-}AsO_4\text{-}H_2O$ (1)	5	**4.829**	"pseudo-voglite"	2	**3.216**	$PbO\text{-}UO_3\text{-}H_2O$
2	**9.047**	$Ca\text{-}(VO)\text{-}AsO_4$	3	**4.806**	"kalium-schröckingerite"	4	**3.214**	$Ca\text{-}(VO)\text{-}AsO_4$
3	**8.835**	"pseudo-voglite"	3	**4.797**	"pseudo-zippeite (Mg)"	3	**3.174**	"pseudo-lindackerite"
2	**8.763**	$Ca_2Cu(UO_2)_2(CO_3)_2O_3$. 3 H_2O	3	**4.758**	$Fe\text{-}AsO_4\text{-}H_2O$(1)	5	**3.127**	"phosphate-walpurgite"
3	**8.716**	$Ca\text{-}Cu\text{-}(UO_2)\text{-}(CO_3)\text{-}H_2O$	1	**4.654**	$Na_4(UO_2)(CO_3)_3$	4	**3.117**	"Mg- villyaellenite"
4	**8.711**	$U(HAsO_4)_2$. 4 H_2O	3	**4.610**	"hydronium uranospinite"	4	**3.101**	$Ca(H_2AsO_4)_2$
4	**8.710**	"hydronium uranospinite"	4	**4.573**	"pseudo-johannite"	5	**3.068**	"pseudo-zippeite (Mg)"
1	**8.548**	$Ni(UO_2)_2(AsO_4)_2$. 6-8 H_2O	5	**4.391**	"Mg- villyaellenite"	5	**3.048**	"pseudo-johannite"
1	**8.228**	$U(HAsO_4)_2$. 4 H_2O	4	**4.380**	$Fe\text{-}AsO_4\text{-}H_2O$(1)	5	**3.041**	$Ca(H_2AsO_4)_2$
3	**8.109**	$Mg\text{-}AsO_4\text{-}H_2O$	4	**4.297**	"kalium-schröckingerite"	5	**2.970**	$Cu\text{-}AsO_4\text{-}H_2O$ (3)
3	**8.071**	$Na_4(UO_2)(CO_3)_3$	2	**4.279**	$Ni(UO_2)_2(AsO_4)_2$. 6-8 H_2O	5	**2.955**	$Ca\text{-}Mg\text{-}AsO_4\text{-}H_2O$
3	**7.944**	$UO_3 - H_2O$ (2)	4	**4.221**	$Fe\text{-}AsO_4\text{-}H_2O$(2)	5	**2.937**	$Cu\text{-}AsO_4\text{-}H_2O$ (1)
2	**7.92**	$Ca\text{-}Mg\text{-}AsO_4\text{-}H_2O$	2	**4.057**	$Mg\text{-}AsO_4\text{-}H_2O$	3	**2.933**	$U(HAsO_4)_2$. 4 H_2O
5	**7.907**	$PbO\text{-}UO_3\text{-}H_2O$	5	**3.983**	$Ca\text{-}Cu\text{-}(UO_2)\text{-}(CO_3)\text{-}H_2O$	2	**2.879**	"kalium-schröckingerite"
4	**7.903**	$PbO\text{-}UO_3\text{-}SO_3\text{-}H_2O$	1	**3.974**	$Ca(H_2AsO_4)_2$	4	**2.852**	"pseudo-zippeite (Mg)"
1	**7.836**	$UO_3 - H_2O$ (1)	5	**3.842**	"hydronium uranospinite"	5	**2.771**	$Mg\text{-}AsO_4\text{-}H_2O$
2	**7.798**	$Cu\text{-}AsO_4\text{-}H_2O$ (2)	5	**3.808**	$Fe\text{-}AsO_4\text{-}H_2O$(1)	2	**2.687**	$Na_4(UO_2)(CO_3)_3$
2	**7.784**	$Cu\text{-}AsO_4\text{-}H_2O$ (1)	5	**3.708**	$PbO\text{-}UO_3\text{-}SO_3\text{-}H_2O$	4	**2.3262**	$Na_4(UO_2)(CO_3)_3$
1	**7.630**	$PbO\text{-}UO_3\text{-}H_2O$	4	**3.649**	"pseudo-lindackerite"	5	**2.1432**	$Ca\text{-}(VO)\text{-}AsO_4$
4	**7.588**	$UO_3 - H_2O$ (2)	5	**3.623**	$UO_3 - H_2O$ (2)	3	**2.1396**	$Ni(UO_2)_2(AsO_4)_2$. 6-8 H_2O
2	**7.406**	$PbO\text{-}UO_3\text{-}SO_3\text{-}H_2O$	3	**3.586**	$Fe\text{-}AsO_4\text{-}H_2O$(2)			

Reflections are sorted according d-spacings. Columns contain intensity (scaled 1-5 with 1 = highest), ***d-spacing*** *and name.*

Nové sekundární minerální fáze z Jáchymova

Tato práce popisuje 30 anorganických sloučenin – sekundárních minerálů - poprvé pozorovaných v přírodě. Všechny látky jsou z jáchymovského rudního revíru.

V práci jsou uvedena doposud známá fyzikálně-chemická data a odkazy na další literaturu. U fáze [$(MoO_2)_2As_2O_5(H_2O)_2$] . H_2O byla vyřešena krystalová struktura, pro fáze $Ca(H_2AsO_4)_2$ a Mg-villyaellenit byly vypřesněny strukturní data Rietveldovou analýzou.

Portal of an old abandoned adit in the Geshieber vein near the church. The beginning of this century.

Miner Josef Prennig who transported radioactive water in a 40-litre wooden vat from the Štěp's sprinsgs in the Werner mine (now Rovnost) through the Daniel drift into the spa situated in a house of baker Kühn. Distance was about 3 km underground and 2 km on the surface. 1906.