

BOOK OF ABSTRACTS



ECMS 2019

**9th European Conference
on Mineralogy and Spectroscopy**

9th European Conference on Mineralogy and Spectroscopy, September 11-13, 2019, Prague, Czech Republic, Břevnov Monastery

One of the real advantages of scientific congresses and conferences is that people can share their ideas and visions, and may find a way to implement them. They serve as useful feedback as well as stimulation of future research. In the past, conferences have also served as a powerful weapon against all boundaries, primarily during the years of the "Iron Curtain" in Europe. We should be glad that no such a curtain exists today; boundaries prevail only in our minds (which is, fortunately, our own struggle only). Following the European Spectroscopic Conferences first held in Rome (1988), then in Berlin (1995), Kiev (1996), Paris (2001), Vienna (2004), Stockholm (2007), Potsdam (2011), Rome (2015), the 9th European Conference on Mineralogy and Spectroscopy (ECMS 2019) is hosted by Prague. Břevnov Monastery, which is now an archabbey, was the oldest male monastery in the Kingdom of Bohemia, founded in 993 and connected with the great personality of Saint Adalbert (956–997). The rule is of Saint Benedict, Ordo Sanctum Benedictum. Since their beginning, monasteries have been the centers of theology, philosophy, education and science. We are delighted that the conference venue combines both great history and great spirit.

The Bohemian countries (historic designation of countries that belonged to the Czech/Bohemian Crown, later on a part of the Austrian Empire) have great and long tradition of mineralogical research, which is primarily connected with the long history of mining ores since the early middle ages, such as Kutná Hora, Jihlava, later on Jáchymov (the origin place of tolar/thaler silver coins, predecessor of dolar) and Příbram. Many great and renowned scientists worked in Bohemian countries. As examples may serve Georg Bauer (known as Georgius Agricolas) (1494–1555), Tadeáš Hájek z Hájku (in Latin known as Hagecius) (1555–1600), Tycho Brahe (1546–1601), Johannes Kepler (1571–1630), Joseph Stepling (1716–1778), Joachim Barrande (1799–1883), Franz Xaver Maximilian Zippe (1791–1863), František Pošepný (1836–1895) and others, namely those who were active during the second half of the 19th century as professors of the Mining Academy in Příbram. The 20th century became providential for great personalities in Czech mineralogy, such as František Slavík (1876–1957), Ludmila Kaplanová-Slavíková (1890–1943), Vojtěch Rosický (1880–1942), František Ulrich (1899–1941), Radim Nováček (1905–1942) and later on Josef Sekanina

(1901–1986), Jiří Novák (1902–1971), Rudolf Rost (1912–1999), Jiří Krupička (1913–2014), Zdeněk Pouba (1922–2011), Karel Paděra (1923–2010), Lubor Žák (1925–2008), Jan Kutina (1924–2008), František Čech (1929–1996) and Petr Černý (1934–2018). While the first half of the century was tragically affected by the two world wars (many of the scientists died, others were imprisoned), the second half was marked by the totalitarian Communist regime (many scientists were persecuted or imprisoned, others were deprived of their jobs). Despite these dire circumstances, scientific activities continued to be stimulated due to an immeasurable effort and often personal credit of the above-mentioned personalities. In the difficult years under the Communist ruling, **Ing. Jiří Čejka, DrSc.** (born 1929 in Roudnice nad Labem) embarked on his scientific career and has had to overcome various obstacles throughout the years. Nowadays, he is a world-renowned expert in the field of vibration spectroscopy of uranium minerals and compounds, and still scientifically active! This year, Jiří Čejka celebrates his **90th birthday**, and, therefore, we decided to dedicate one of the scientific sessions focused on Uranium mineralogy to him and also symbolically dedicate the entire conference to his honor. We are convinced that Jiří is the best representative of an interdisciplinary approach in science as he is originally a chemist, who has

gradually fallen in love with uranium mineralogy and spectroscopy. This is more than characteristic for interdisciplinary nature of the ECMS conferences, as from their beginning. We hope you will enjoy the great hospitality of Prague with its sightseeing and history, as well as the stimulating atmosphere of the conference!

On behalf of the Scientific Committee
Jakub Plášil

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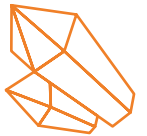


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CONFERENCE SCHEDULE



	9/9	9/10	9/11	9/12	9/13	9/14		
8.00–9.00			Participant registration					
9.00–9.40	Workshop I (Jana 2006)	Workshop I (Jana 2006)	Conference opening	Keynote lecture	Keynote lecture	Workshop II (Gemstone deposits)		
			Keynote lecture					
9.40–10.40			Talks	Talks	Talks			
10.40–11.10			Coffee break	Coffee break	Coffee break			
11.10–12.40			Talks	Talks	Talks			
12.40–14.00			Lunch break	Lunch break	Lunch break			
14.00–14.40			Keynote lecture	Keynote lecture	Keynote lecture			
14.40–15.25			Talks	Talks	Talks			
15.25–15.45			Coffee break	Coffee break	Coffee break			
15.45–16.45					Talks		Talks	Talks
					Summary & closing			
16.45–18.00			Ice-breaker party (17.00–19.00)		Poster session		Poster session	
18.00–19.00					Poster session			
19.00–24.00					Conference dinner			

A new solvothermal approach to obtain nanoparticles in the Cu_3SnS_4 - $\text{Cu}_2\text{FeSnS}_4$ join

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In the field of the renewables, a large effort has been devoted in the last years to obtain conventional and new materials for solar energy conversion by using methods which couple a good efficiency and scalability with energetic and environmental concerns. This research has obviously included the so-called kesterites, materials considered interesting for the thin film solar cell technology, which consists of relatively abundant and harmless elements: $\text{Cu}_{3-x}\text{Fe}_x\text{Zn}_y\text{Sn}(\text{S},\text{Se})_4$.

In this study, we undertook the synthesis of terms of the kuramite-stannite (Cu_3SnS_4 - $\text{Cu}_2\text{FeSnS}_4$) join by means of a two-step solvothermal approach, which is able to provide nanocrystalline products in an easy, low temperature, and fast way.

The sample with the highest Fe concentration was characterised by means of a multi-analytical approach, aimed to assess not only its final structural, chemical and micromorphological features, but also the redox speciation of the two transition metal cations, i.e. Cu and Fe, in relation to the overall charge balance. Namely, EPR, Mössbauer and XAS spectroscopies and SQUID magnetometry were involved.

The main results point out an excellent control of the structural features, and a good Fe content in the sample, leading to the following formula unit: $\text{Cu}_{1.9}\text{Fe}_{0.6}\text{SnS}_4$. According to this composition, a relevant fraction of oxidised Cu and Fe ions were hypothesized. The overall finding of the multi-analytical characterisation point to a complex redox balance, where inferring the site occupancy is non trivial: the charge balance, in fact, can only be achieved taking into account the presence of both Cu(II) and Fe(III) but also vacancies; moreover, Fe is distributed over two different crystallographic sites.

Arsenic in roméite-group minerals formed by weathering of realgar-rich tailings (Lojane mine, North Macedonia)

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Realgar and stibnite are the primary sources of arsenic and antimony contamination of the soils and water at the Sb-As-Cr Lojane mine (abandoned since 1979) in North Macedonia. The waste material comprises various waste dumps, an unprotected flotation tailings dump, and waste from a smelter. We have studied the association of As and Sb in realgar and stibnite weathering products from material sampled at the subsurface of the realgar-rich (up to 60 wt% realgar), fine-grained (20 to 100 μm) and porous tailings which contain significant amounts of stibnite (up to 13.5 wt%) [1].

Besides minor scorodite, arsenolite, annabergite, native sulfur, iron oxy-hydroxides, pickeringite, and alunogen, the weathering of the tailings material produces a chemically inhomogeneous Sb-As-Fe-Ca-(Ni)-oxide/hydroxide as the most widespread secondary phase. In this phase the As:Sb ratio varies from ca. 2:1 to 1:2.2 and the Fe content is variable. The phase mostly forms thin coatings around realgar and stibnite grains, but Sb-dominant variants also form larger homogeneous grains up to 500 μm , characterized by broad dehydration cracks.

Using a combination of SEM-EDS, TEM, and Raman spectroscopy, this poorly crystalline to amorphous weathering product was determined to be an (often As-dominant) member of the roméite-group minerals (RGM) which themselves belong to the large pyrochlore supergroup of minerals [2] with general stoichiometry $\text{A}_2\text{B}_2\text{X}_6\text{Y}$, where A = non-framework cations (ideally 8-coordinated), B = octahedrally coordinated framework cations, X = framework anions and Y = non-framework anions. Although B sites are likely to be fully occupied, A sites may be partially vacant. The total number of cations per formula unit depends on valence determination, as does the amount of H needed for charge balance, and hence minimum H_2O content.

The crystallographic position of arsenic in the RGM in our samples is not fully clear. Although As^{5+} may occupy the octahedrally coordinated B-position in the roméite structure, it strongly prefers a tetrahedral coordination. The distorted A-centered polyhedron in RGM is too large for the As^{5+} cation. These crystal-chemical preferences explain that the As is hosted mostly in the X-ray amorphous phases. However, EDS point analyses clearly document that the roméite-type phase may incorporate considerable arsenic. Besides the intense Raman band at $\sim 520\text{ cm}^{-1}$ assigned to the Sb-O symmetric stretching mode and the band at $\sim 466\text{ cm}^{-1}$ assigned to the Sb-O antisymmetric stretching mode, Raman spectra of RGM-phases show additional weaker and broader bands in the region $835\text{--}915\text{ cm}^{-1}$. These bands correspond to the AsO_4 stretching vibrations [3] and thus additionally confirm the presence of As^{5+} in the structure.

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References

- [1] Dordević, T., et al. (2019) *Can. Mineral.* 57, 1–21.
- [2] Bosi, F., et al. (2017) *Mineral. Mag.* 81, 1287–1302.
- [3] Bahfenne, S., et al. (2010) *Appl. Spec. Reviews* 45, 101–129.