

MS15-P04**Evolution of uranyl-bearing structural complexes**Vladislav Gurzhiy¹, Sergey Krivovichev¹

1. St. Petersburg State University, Crystallography Dept., St. Petersburg, Russia

email: vladgeo17@mail.ru

Uranyl sulfates and selenates are the most remarkable groups of U⁶⁺-containing compounds due to their mineralogical importance and fascinating variety of structural topologies and topological isomers. The unique diversity of these materials can be explained by the high topological and structural adaptability of uranyl-based structural units to the charge and shape of organic and/or inorganic complexes that compensate for the negative charge of the uranyl complexes. Due to the small energetic differences between distinct topologies with the same overall composition, the structures of uranyl-based units may adapt to a particular template through topological and geometrical variations, thus demonstrating considerable structural flexibility. The interesting problem that appears in this regard is how complexity of a particular topological structure is related to the shape and complexity of templating ions.

Within the conceptual framework of the information-based approach, uranyl-containing 1D and 2D units have been investigated using topological approach and information-based complexity measures demonstrating that very complex structures may form as transitional architectures between phases with relatively small amounts of structural information [1], wherein the overall trend shows that complexities of structures formed on the latter stages of crystallization are higher than those for the phases growing on the primary stages [2]. In addition, it was found that complex topologies form more rare than their simplest counterparts, which is a response of the crystal structure to changes of chemical conditions within the system [3].

This work was supported by St. Petersburg State University, President of Russian Federation grant for young scientists (no. MK-4810.2018.5) and Russian Science Foundation (no. 18-17-00018).

References:

- [1] Gurzhiy, V.V., Tyumentseva, O.S., Krivovichev, S.V., Krivovichev, V.G., Tananaev I.G. (2016) *Cryst. Growth Des.*, 16, 4482-4492.
 [2] Gurzhiy, V.V., Krivovichev, S.V., Tananaev I.G. (2017) *J. Solid State Chem.*, 247, 105-112.
 [3] Gurzhiy, V.V., Tyumentseva, O.S., Krivovichev, S.V., Tananaev I.G. (2018) *Z. Kristallogr.* 233, 233-245.

Keywords: Uranyl, crystal structure, structural complexity**MS15-P05****Structural diversity of terrestrial phosphides related to Fe-Ni-P system**Maria Krzhizhanovskaya¹, Sergey Britvin¹, Michail Murashko¹, Yevgeny Vapnik², Andrey Zolotarev¹

1. Department of Crystallography, Institute of Earth Sciences, Saint-Petersburg State University, St. Petersburg, Russia

2. Ben-Gurion University of the Negev, Beer-Sheva, Israel

email: krzhizhanovskaya@mail.ru

The recent findings of terrestrial phosphides related to Fe-Ni-P triangle (Table 1) substantially expand our knowledge on this important cosmochemical system. We herein provide comparative crystal chemical characteristics of terrestrial phosphides vs. their counterparts of space origin. Crystal structures of some of the listed minerals are studied by both single crystal and powder X-ray diffraction. Special attention has been paid to the distribution of iron and nickel in their structures. The possibility of X-ray diffraction approach, involving anomalous scattering of CoK α -radiation at the Fe-K edge, is discussed.

Table 1. Natural phosphides in the Fe-Ni-P system

Mineral	Formula	Structural type
<i>Negevite</i>	NiP ₂	Pyrite
<i>Zuktamrurite</i>	FeP ₂	Marcasite
<i>Murashkoite</i>	FeP	FeP
<i>Halamishite</i>	Ni ₅ P ₄	Ni ₅ P ₄
<i>Transjordanite</i>	Ni ₂ P	Fe ₂ P
Barringerite	Fe ₂ P	Fe ₂ P
Allabogdanite	(Fe,Ni) ₂ P	Co ₂ Si
Nickelphosphide	(Ni,Fe) ₃ P	Ni ₃ P
Schreibersite	Fe ₃ P	Ni ₃ P
Melliniite	(Ni,Fe) ₄ P	Cr ₄ Si

* The names of new phosphide minerals are highlighted by italic.

This study was carried out under financial support of Russian Scientific Foundation, grant no. 18-17-00079. The authors thank the Center for X-ray Diffraction Studies and Geomodel Center of Saint-Petersburg State University for instrumental and computational support.

Keywords: phosphides, crystal structure, mineral