MS14-02 | New Data about Topology and Modularity of Heteropolyhedral Frameworks in Minerals and Inorganic Compounds

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Zeolites compose an important class of inorganic crystalline materials that have been widely used in technology. A family of microporous materials demonstrates that frameworks can be built by TO_4 tetrahedra and MO_6 octahedra (*M* – predominantly transitional metals: Ti, Nb, Zr, Sn, Fe, Mn, etc.). Such heteropolyhedral zeolite-like materials are also characterized by many useful physical and chemical properties and attract interest (especially titanium silicates) as ion-exchangers because of their efficient absorption of heavy elements from aqueous solutions.

The modern topological analysis of zeolite structures using the ToposPro software is based on the types of linkage of natural tiles, the smallest tetrahedral clusters, to form a framework structure. In this case, it can be also useful to characterize a topology of the heteropolyhedral frameworks as they represent the same 3D cationic nets.

Another way for describing complex structures of minerals and inorganic compounds is the modular approach, when the structure is described as a combination of a number of fragments – modules. It is closely related to the concepts of order/disorder (OD) structures and polysomatic series.

Both approaches have been recently applied for the analysis of hybrid lanthanide-based silicates, uranyl germanates and vanadates, and series of minerals and related compounds with heteropolyhedral frameworks. The relationships between such heteropolyhedral frameworks and tetrahedral framework types were found and described in details and hypothetical zeolite-type materials were predicted.