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Dehydration-Driven Evolution of Topological Complexity in Ethylammonium Uranyl Selenates

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Abstract

Single crystals of four novel uranyl selenate and selenite-selenate oxysalts with protonated ethylamine molecules, $(\text{C}_2\text{H}_8\text{N})_2[(\text{UO}_2)(\text{SeO}_4)_2(\text{H}_2\text{O})](\text{H}_2\text{O})$ (**I**), $(\text{C}_2\text{H}_8\text{N})_3[(\text{UO}_2)(\text{SeO}_4)_2(\text{HSeO}_4)]$ (**II**), $(\text{C}_2\text{H}_8\text{N})[(\text{UO}_2)(\text{SeO}_4)(\text{HSeO}_3)]$ (**III**), and $(\text{C}_2\text{H}_8\text{N})(\text{H}_3\text{O})[(\text{UO}_2)(\text{SeO}_4)_2(\text{H}_2\text{O})]$ (**IV**) have been prepared by isothermal evaporation from aqueous solutions. Uranyl-containing 1D and 2D units have been investigated using topological approach and information-based complexity measurements that demonstrate the evolution of structural units and the increase of topological complexity with the decrease of H_2O content.

Graphical abstract

Single crystals of four novel uranyl selenate and selenite-selenate oxysalts with protonated ethylamine molecules have been prepared by isothermal evaporation from aqueous solutions. Structural analysis and information-based topological complexity calculations points to the possible sequence of crystalline phases formation, showing both topological and structural branches of evolution.

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