

Recurrent Modules in Modular Structures

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Modular structures are based on complex structural fragments (modules) that occur in different crystal structures. Let A and B be bidimensional and crystal-chemically different modules; A_mB_n represents a polysomatic series formed by members based on different m/n ratios. The cell parameters and chemical composition of the members linearly depend from those of the building modules.

A survey of polysomatic structures recently reported in [1] shows a large variety of recurrent modules. In oxygenated compounds, among others, the following modules recur: bafertisite, brucite, corundum, epidote, gibbsite, mica, nasonite, nolanite, palmierite, perovskite, pyrochlore, pyroxene, rutile, schafarzikite, spinel, talc, and topaz. Tetrahedral (T) and octahedral (O) modules are widespread in nature both as TOT and TO slices; slices of perovskite with various thickness and orientation are present in hundreds of synthetic inorganic materials, including superconductors, and are the basis of several series of inorganic-organic hybrids.

The concept of modularity is a powerful tool increasingly used to handle various crystal-chemical aspects of the structures: (i) modelling the unknown structure of new members of a series; (ii) interpreting topotactic reactions and defects in real structures; (iii) tuning the properties of synthetic materials; (iv) inspiring the synthesis of mesoporous (e.g., pillared clays) and intercalation materials.

[1] Ferraris G., Makovicky E., Merlino S., *Crystallography of Modular Materials*, 2004.

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