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Real structure investigations on oxonitridosilicates $\text{MSi}_2\text{O}_2\text{N}_2$ (M = Ca, Sr, Ba, Eu)

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Nitridosilicates and oxonitridosilicates have gained significant relevance as host lattices in rare-earth-doped phosphors for LED applications [1]. However, the structural characterization of some of these compounds proved to be difficult due to pronounced real structure effects. In addition to stacking disorder and twinning with domains of various sizes, the pseudosymmetry of parts of the structures gives rise to numerous kinds of intergrowth and antiphase domain structures. For example, the triclinic structure of $\text{EuSi}_2\text{O}_2\text{N}_2$ ($P1$, $a = 7.095 \text{ \AA}$, $b = 7.246 \text{ \AA}$, $c = 7.256 \text{ \AA}$, $\alpha = 88.69^\circ$, $\beta = 84.77^\circ$, $\gamma = 75.84^\circ$, $Z = 4$, solved from a twinned crystal) consists of nitridosilicate layers different from those in the Ca compound [2] with terminal O atoms forming an almost tetragonal square net. They alternate with pseudo-hexagonal Eu layers exhibiting pseudotranslational symmetry. Even in apparently ordered samples with minimal diffuse scattering, manifold faults have been detected by HRTEM. The corresponding Sr compound is "isotypic", however, it shows a much higher tendency not to form ordered crystals and presents interesting kinds of multiple intergrowth. A general approach towards a unified description of the disorder present will be given.

[1] Mueller-Mach R., Mueller G., Krames M.R., Höpfe H.A., Stadler F., Schnick W., Juestel T., Schmidt P., *Phys. Status Solidi A* 2005, 202, 1727.

[2] Höpfe H.A., Stadler F., Oeckler O., Schnick W., *Angew. Chem. Int. Ed.* 2004, 43, 5540.

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Crystallochemical analysis of inorganic salts with pyramidal anions $\text{M}_y(\text{LO}_3)_z$ (L = S, Se, Te, Cl, Br, I)

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A comparative crystallochemical analysis and classification are performed for 61 salts $\text{M}_y(\text{LO}_3)_z$ (L = S, Se, Te, Cl, Br, I) containing isolated pyramidal anions LO_3 (simple sulfites, selenites, tellurites, chlorates, bromates, iodates), and 1835 binary compounds A_xB_y using the computer program *IsoTest* of the *TOPOS* software package. The topological similarities between ionic nets in 30 ternary salts $\text{M}_y(\text{LO}_3)_z$ and the six topological types of compounds A_xB_y (NaCl, NiAs, PoCl_2 , Ti_2S_2 , ZnTe, rutile) were first found and discussed. In these relations any ternary salt $\text{M}_y[\text{LO}_3]_z$ was considered as a quasi-binary compound $\text{M}_y[\text{L}]_z$ keeping the connectivity of initial net. Many of the found correspondences are typical also for other anhydrous inorganic salts: with triangular (borates, carbonates, nitrates) and tetrahedral anions (orthophosphates, sulfates, selenates, perchlorates, orthoarsenates, molybdates, halogenides of *d*-metals).

Topological analysis of ionic arrays shows that in 36 out of the 61 salts there are arrays having b.c.c., h.c.p or f.c.c. topology. In most cases a complete cationic array have significant structure-forming role. Using the data on uniformity and topology of these arrays the conclusions are made about influence of the nature of the M and L atoms on the structure-forming role of all ionic constituents of the $\text{M}_y(\text{LO}_3)_z$ crystal structures.