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Structural filiations in the new SrLiMTi$_4$O$_{11}$ (M= Cr, Fe) titanates

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Titanates occupy an important place among advanced oxide materials. After characterization of M^{II}Li$_2$Ti$_6$O$_{14}$ compounds in the ternary oxide systems MO - Li$_2$O - TiO$_2$ (M = Sr, Ba, Pb) [1],[2], two new titanates of Sr, Li and a 3d transition metal, SrLiM^{III}Ti4O11 (where M = Cr, Fe) were discovered. Single crystals were obtained by spontaneous nucleation using LiBO$_2$ as flux. The SrLiCrTi$_4$O$_{11}$ structure was refined using 1491 independent reflections in orthorhombic space group *Pmna*, with a=13.818Å, b=5.755Å, c=9.901Å, Z=4, R$_1$=0.021 and wR$_2$=0.058. The SrLiFeTi$_4$O$_{11}$ structure was refined using 5005 independent reflections in orthorhombic space group *Pbcn*, with a=13.878Å, b=11.496Å, c=19.895Å, Z=16, R$_1$=0.036 and wR$_2$=0.105. Structures can be described by the close-packed arrangement of strontium and oxygen atoms. The unit cell contains 6 ”compact planes” perpendicular to [100] in the layer sequence ABACBC ((chc)$_2$). Titanium, chromium or iron atoms occupy some of the created interstitial octahedral sites whereas lithium atoms are situated in tetrahedral sites. Depending on the synthesis conditions of SrLiCrTi$_4$O$_{11}$, the chromium and titanium atom distributions over the four allowed crystallographic sites are not the same. Having a similar compact-planes sequence, SrLiCrTi$_4$O$_{11}$ and SrLiFeTi$_4$O$_{11}$ structures differ in the arrangement of strontium and oxygen atoms per layer of close packing which also induces correlated variation in the Li-tetrahedra distribution.

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Synthesis and structure of a cerium succinato-bridged ionic open-framework

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The area of hybrid open-framework materials based on carboxylate function, is currently of great interest owing to their features inducing catalytic and sorption properties. Their zeolite-like catalytic reactivity is a relatively recent attribute due probably to their crystalline nanoporous character.

Moreover, the flexibility of aliphatic dicarboxylic ligands, associated with connectivity of rare-earth metals, offer a great variety of coordination polymers extended into 1D, 2D or 3D via coordination bonding.

The hydrated cerium succinate, crystallizing with a counter ion (Cl$^-$) has been obtained by an indirect synthetic route under reflux. Single crystals X-ray diffraction studies have been carried out at both room temperature (293K) and low temperature (120K).

Isostructural with the precedent lanthanum (III) succinate [1], it forms a layer-type polymeric structure built up from infinite Ce-O-Ce chains and self-assembled succinate ligands. The Ce atoms are ten-fold coordinated by six oxygen atoms of two symmetrically equivalent succinate ligands and four crystallographically distinct aqua ligands, to form edge-shared Ce O$_6$(H$_2$O)$_4$ bicapped square antiprism. The two end functional groups of the succinate ion are involved in the same syn-anti bridging-chelating mode and link the metal atoms through μ_2-oxo bridges.

The hydrogen bonds crosslink the cationic layers into a 3 D open-framework and keep in place discrete chloride anions, and lattice water molecules.

As well as the lanthanum compound, [Ce(C$_4$H$_4$O$_4$)(H$_2$O)$_4$.3H$_2$O].Cl has high thermal stability and exhibits the same thermal behaviour. The removal of all lattice water molecules and three from four coordinated ones occurs in the temperature range 53-220°C and gives an intermediate anhydrous compound stable up to 320°C.

The heavier lanthanides (Nd and heavier) are often isostructural [2][3]. Besides, lanthanum and cerium are also isostructural, pointing to the influence of metal ion size and lanthanide contraction upon the structure, in this kind of materials.

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