m39.p06

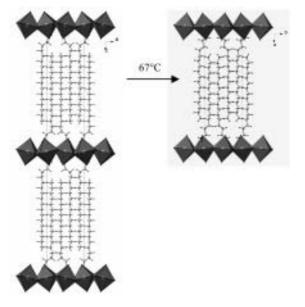
Temperature Dependant Phase Transitions of Organic-Inorganic Hybrid Perovskites

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Keywords: phase transitions, organic-inorganic hybrids, thermochromism

The basic building components of the organic-inorganic perovskite family include slices or cuts of the ABX₃ perovskite structure, which consists of MX₄²-layers of corner-sharing metal halide octahedra alternating with A²⁺ amine cation bilayers (for monofunctional cations) or monolayers (for bifunctional cations). The $(C_nH_{2n+1}NH_3)_2PbI_4$ materials often exhibit a range of temperature-dependant structural transitions as a result of changes in the ordering and hydrogen bonding of the organic cations, as well as thermochromic behaviour. These transitions where investigated using Single Crystal Diffraction, Differential Scanning Calorimetry and Hot Stage Microscopy to elucidate the mechanism and exact structural changes. The structural phase transitions observed can be divided into two classes: Order-disorder transitions of the rigid alkyl ammonium chains, and conformational transitions of the chains and octahedral layers. The most obvious effect is a change in the crystal setting of the structure. For the series n = 12, 14, 16 and 18, the following sequence is observed: The unit cell at room temperature is orthorhombic (ORT) and contains three layers. Upon heating, the unit cell halves and transforms to a monoclinic system with only two layers in the unit cell. In the ORT phase, the octahedra in the inorganic layers are staggered relative to each other and more corrugated in one direction. The monoclinic high temperature phase (MHT) now has an eclipsed geometry of the layers.



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Hydrothermal Synthesis and Crystal Structure of a new family of Lanthanide Phosphonates: [H₃N(CH₂)₄NH₃]Ln[hedpH₂] [hedpH]

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Keywords: structural characterization, phosphonates, hydrothermal synthesis

One-dimensional (1D) nanostructures have recently gained interest and importance based on their novel properties associated with the reduced dimensionality and their potential applications in nanotechnology. Hydrothermal methods have been extensively used in the synthesis of 1D nanomaterials. Hereby we report the hydrothermal synthesis and structural characterization of a new family of isostructural 1D lanthanide phosphonates. The general formula of all compounds is [H₃NCH₂CH₂CH₂CH₂NH₃]Ln[hedpH₂][hedpH], hedpH₂ and hedpH are two deprotonated forms of the diphosphonic acid [H2O3PCCH3OHPO3H2] and Ln is a trivalent lanthanide metal (Ln=La,Pr,Sm,Tb,Er). They crystallize in space group P-1, and the cell parameters change slightly with the trivalent lanthanide cation radii. The cell parameters of the La-phosphonate crystal are: a=10.215Å, b=10.697Å, c=10.722Å, $\alpha=67.48^{\circ}$, $\beta=89.98^{\circ}$, and $\lambda=68.65^{\circ}$.