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Structural versus electrical properties of an organic-inorganic hybrid material based on sulfate.

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ABSTRACT

A new organo-sulfate compound is obtained by slow evaporation at room temperature and is characterized by powder and single-crystal X-ray diffraction (XRD) at variable temperatures. The benzylammonium monohydrogenosulfate of formula $C_6H_5CH_2NH_3^+ \cdot HSO_4^-$, denoted (BAS), crystallizes in the monoclinic system $P2_1/c$ space group with the following parameters at room temperature : $a = 5.623(5)\text{\AA}$, $b = 20.239(5)\text{\AA}$, $c = 8.188(5)\text{\AA}$, $\beta = 94.104(5)^\circ$. The crystal structure consists of infinite parallel two-dimensional planes built by HSO_4^- anions and $C_6H_5CH_2NH_3^+$ cations interconnected by strong O–H....O and N–H....O hydrogen bonds. A phase transition is detected at 350 K by differential scanning calorimetry (DSC) and confirmed by powder XRD. Conductivity measurements using the impedance spectroscopy technique allow to determine the conductivity relaxation parameters associated with the H^+ conduction from an analysis of the M''/M''_{max} spectrum measured in a wide temperature range. Transport properties of this material appear to be due to an H^+ ion hopping mechanism.

Graphical abstract

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