MS15-P14 Structure, dielectric and electric properties of diisobutylammonium hydrogensulfate crystals

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The $[(CH_3)_2CHCH_2)_2NH_2][HSO_4]$ (abbreviated as **dibahs**) salt was obtained from 1:1 mixture of diisobutylamine (99%, Sigma-Aldrich) and 30% aqueous solution of sulfuric acid (purum, Sigma-Aldrich). Single crystals were grown by slow evaporation of water at room temperature. DSC studies have revealed two high-temperature reversible phase transitions at 336/319 K (**III→II**) and 339/337 K (**II→I**), respectively for heating/cooling cycles. Single-crystal X-ray diffraction data were collected at room temperature (phase **III**), after heating to 360 K (phase **I**) and after cooling to 335 K (phase **II**). At room temperature **dibahs** crystallizes in the triclinic symmetry (space group *P*-1). Its crystal structure is built of isolated ordered diisobutylammonium cations (**diba**) and hydrogensulfate anions (**hs**) arranged into layered crystal packing. On heating dibahs transforms into monoclinic space group $P2_1/c$ and the transition (**III→II**) may be classified as both of "order–disorder" and of "displacive" one and related to a disorder of the **diba** cations and a reorientation of the inorganic sublattice. The second transition (**II→I**) is followed by a change in the symmetry to orthorhombic space group *Cmce* and caused by an increase in the disorder in organic sublattice and a small deformation. As-grown single crystals of **dibahs** are usually single domain and ferroelastic domains were found to appear at room temperature due to application of a small mechanical stress. Evolution of the ferroelastic domain pattern was measured on heating and on cooling. Dielectric response and ac conductivity were measured for pellets (powder pressed at 600 MPa) with gold evaporated electrodes using an Alpha-A High Performance Frequency Analyzer (Novocontrol GmbH) combined with Quatro Cryosystem for the temperature control. The Figure below shows temperature variation in dielectric permittivity *e'* and electric conductivity *s'* at various frequencies. The dielectric anomalies are related to changes in the electric conductivity. The activation energy E_a was calculated for dc conductivity (1Hz) and in the range: 413 K< T <435 K → E_a = 1.78 eV, 356 K< T <395 K → E_a = 0.23 eV, 335 K< T <341 K → E_a = 1.51 eV. The low activation energy of 0.23 eV in the temperature range between ~356 K and ~395 K can be to ascribed to fast transport of the acid proton in the lattice of **dibahs** crystals.

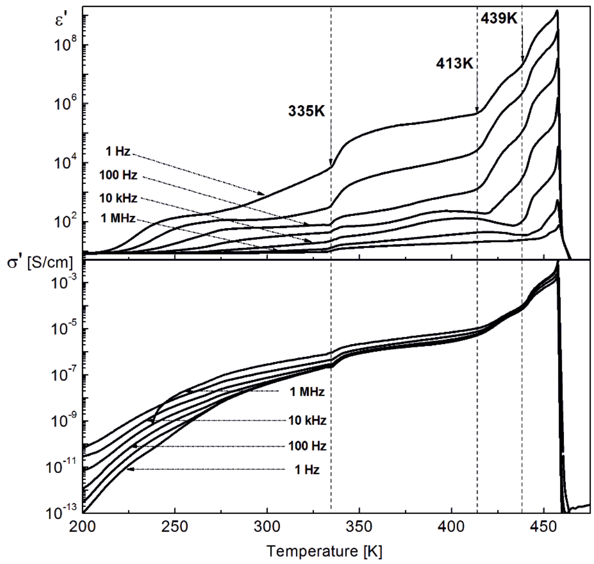

Figure 1.

Keywords: crystal structure, phase transitions, ferroelastic, dielectric and electric properties