

Synthesis, crystal structure and phase transitions of a series of imidazolium iodides.

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Streszczenie

The reaction of imidazole with hydroiodic acid leads to three products crystallizing as ionic salts; $[C_3N_2H_5 +][I_2]$, $[C_3N_2H_5 +]_2[I_4 22]$ and $[C_3N_2H_3I_2 +][I_2]$. All the analogs were characterized by single-crystal X-ray diffraction, while the first two were additionally studied by calorimetric, dilatometric, dielectric and proton magnetic resonance methods. At room temperature (RT), $[C_3N_2H_5 +][I_2]$ adopts the centrosymmetric, trigonal space group ($R\bar{3}$). The crystal structure consists of disordered imidazolium cations and discrete I_2 ions. $[C_3N_2H_5 +]_2[I_4 22]$ undergoes two discontinuous phase transitions (PTs) at 180/185 K and 113/ 123 K (cooling–heating), both of them governed by the imidazolium cation dynamics. $[C_3N_2H_5 +]_2[I_4 22]$ consists of disordered imidazolium cations and quite rare and exotic $[I_4] 22$ tetraiodide counterion. It undergoes continuous PT at 204 K of the ferroelastic type with a symmetry change from orthorhombic $Fddd$ to monoclinic $C2/c$. The mechanism of PT is complex and consists of ‘order–disorder’ and ‘displacive’ contributions that are assigned to the dynamics of cations and to the distortion of the $[I_4 22]$ rods, respectively. $[C_3N_2H_3I_2 +][I_2]$ is built up of discrete 4,5-diiodoimidazolium cations and isolated I_2 ions. A characteristic feature of this compound is the presence of a layered structure in which moieties are held together by strong $I\dots I$ halogen interactions and $N-H\dots I$ hydrogen bonds.

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