



Unprecedented transformation of $[I^- \cdot I_3^-]$ to $[I_4^{2-}]$ polyiodides in the solid state : structures, phase transitions and characterization of dipyrazolium iodide triiodide.

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Streszczenie

Dipyrazolium iodide triiodide, $[C_3N_2H_5^+]_2[I^- \cdot I_3^-]$, has been synthesized and studied by means of X-ray diffraction, differential scanning calorimetry, dielectric measurements, and UV-Vis spectroscopy. Two reversible, solid–solid phase transitions (*Imma* (I) $\leftrightarrow$ (II) $\leftrightarrow$ *Pbam* (III)) at 254 K and 182/188 K respectively have been revealed. The anionic network experiences spectacular changes associated with a huge rebuilding of the inorganic network from $[I^- \cdot I_3^-]$ to $[I_4^{2-}]$. The low frequency dielectric relaxation process occurs in phase II with the activation energy of ca. 34 kJ mol⁻¹. The molecular motion of the pyrazolium cations in $[C_3N_2H_5^+]_2[I^- \cdot I_3^-]$ has been studied by means of proton magnetic resonance studies (¹H NMR). The ferroelastic properties of all phases have been confirmed by polarizing microscopy observations. The molecular mechanism of the phase transitions in the compound is proposed.

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