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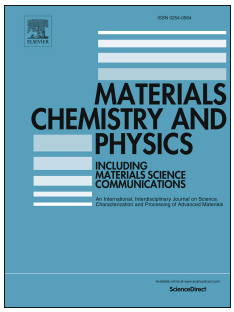

Discontinuous transition from insulator to semiconductor induced by phase change of the new organic- inorganic hybrid $[(CH_2)_7(NH_3)_2]CoBr_4$

Mohga F. Mostafa, Shimaa S. Elkhiyami, Seham A. Alal

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Discontinuous transition from insulator to semiconductor induced by phase change of the new organic- inorganic hybrid $[(CH_2)_7(NH_3)_2]CoBr_4$

Mohga F. Mostafa*, Shimaa S. Elkhiyami, Seham A. Alal†

Physics Department, Faculty of Science, University of Cairo, Giza, Egypt

Abstract

$[(CH_2)_7(NH_3)_2]CoBr_4$, triclinic crystal has a space group $P\bar{1}$ with two molecules per asymmetric unit cell (Z = 2). Unit cell dimensions are: a = 7.6588 (3) Å, b = 10.5160 (3) Å, c = 11.3319 (5) Å, α = 66.745 (2) °, β = 77.2258 (13) °, γ = 88.001 (2) °, volume = 816.37(5) $Å^3$ and calculated density = 2.078 Mgm^{-3}. The structure consists of $[CoBr_4]^{2-}$ tetrahdera separated by heptane diammonium layers. The organic hydrocarbon layers' pack in a stacked herring-bone manner hydrogen bonded to the halide ions. Lattice potential energy is U_{pot} = 1827.7 kJ/mol, and molecular volume V_m= 0.408 nm^3. Calorimetric (DSC) measurements indicate phase transitions at T_1=350±1 K (ΔS = 22.7 J/K-mol) and 335 K (ΔS =10.5 J/K-mol). Dielectric and conductivity as a function of temperature (300<T K< 420) and frequency (0.21 < f (kHz) < 60) were investigated. Abrupt change from an insulator to semiconductor behavior takes place around T_1. At low temperatures, thermally activated Arrhenius behavior is observed with frequency dependent, temperature independent activation energy. At high temperatures conductivity and activation energy are frequency and temperature dependent implying non-Arrhenius type behavior where the charged particles experience different potentials for local and long distance movements. Conduction takes place via correlated barrier hopping with maximum barrier height W_M= 0.015 eV.

Key words: X-ray crystal structure, Phase transition, Dielectric constant, conductivity.
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*Corresponding author: e-mail: Mohga40@Yahoo.com

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