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M.F. Mostafa, ShS. El-khiyami, S.K.A. Elal

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Structure, thermal, and impedance study of a new organic–inorganic hybrid $[(CH_2)_7(NH_3)_2]CoCl_4$

M.F. Mostafa*, Sh.S. El-khiyami, S. K. A. Elal†

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

Abstract

[(CH₂)₇(NH₃)₂]CoCl₄ crystallizes in the triclinic system, space group P-1 with two molecules per asymmetric unit cell (Z=2). The unit cell dimensions are a=7.3107 (2) Å, b=10.1841 (3) Å, c=11.2690 (4) Å, $\alpha=66.81(2)$, $\beta=78.85$ (12), and $\gamma=87.66(2)$. The unit cell volume and the calculated density are 756.11 (4) Å³ and 1.463 Mg m⁻³, respectively. The structure of the hybrid is characterized by alternating layers of inorganic [CoCl₄]²⁻ anion and heptane diammonium cation. The organic hydrocarbon layers are packed in a stacked herring-bone manner with hydrogen bonds to the halide ions. The lattice potential energy U_{pot} and the cation molecular volume V⁺ are 1856.2 kJ/mol and 0.37 nm³, respectively. DSC showed a compound (broad) peak at T₁=331 K, T₂=328 K with total entropy Δ S = 36.2 J/K. mol, and a λ -like endothermic peak at T₃=296 K (Δ S = 24.9 J/K. mol). Dielectric properties are investigated at different temperatures and frequencies [260 K < T < 360 K and 0.06 kHz < f < 60 kHz, respectively]. Super-linear power law is observed for the AC conductivity, which is analyzed based on the jump relaxation model.

Key words: Conductivity; Dielectric constant; Phase transition; X-ray crystal structure.

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*Corresponding author: e-mail: Mohga40@Yahoo.com

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