

A New Co(II) Metal Complex Template with 4-dimethylaminopyridine Organic Cation: Structural, Hirshfeld Surface, Phase Transition, Electrical Study and Dielectric Behavior

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Abstract : Great attention has been paid to the design and synthesis of novel organic-inorganic compounds in recent decades because of their structural variety and the large diversity of atomic arrangements. In this work, the structure for the novel dimethyl aminopyridine tetrachlorocobaltate $(C_7H_{11}N_2)_2CoCl_4$ prepared by the slow evaporation method at room temperature has been successfully discussed. The X-ray diffraction results indicate that the hybrid material has a triclinic structure with a P space group and features a 0D structure containing isolated distorted $[CoCl_4]^{2-}$ tetrahedra interposed between $[C_7H_{11}N_2]^+$ cations forming planes perpendicular to the c axis at $z = 0$ and $z = \frac{1}{2}$. The effect of the synthesis conditions and the reactants used, the interactions between the cationic planes, and the isolated $[CoCl_4]^{2-}$ tetrahedra are employing N-H...Cl and C-H...Cl hydrogen bonding contacts. The inspection of the Hirshfeld surface analysis helps to discuss the strength of hydrogen bonds and to quantify the inter-contacts. A phase transition was discovered by thermal analysis at 390 K, and comprehensive dielectric research was reported, showing a good agreement with thermal data. Impedance spectroscopy measurements were used to study the electrical and dielectric characteristics over a wide range of frequencies and temperatures, 40 Hz-10 MHz and 313-483 K, respectively. The Nyquist plot (Z'' versus Z') from the complex impedance spectrum revealed semicircular arcs described by a Cole-Cole model. An electrical circuit consisting of a link of grain and grain boundary elements is employed. The real and imaginary parts of dielectric permittivity, as well as $tg(\delta)$ of $(C_7H_{11}N_2)_2CoCl_4$ at different frequencies, reveal a distribution of relaxation times. The presence of grain and grain boundaries is confirmed by the modulus investigations. Electric and dielectric analyses highlight the good protonic conduction of this material.

Keywords : organic-inorganic, phase transitions, complex impedance, protonic conduction, dielectric analysis

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