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Electrical resistivities and activation energies of diphenylpyraline hydrochloride complexes

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Abstract : The resistivity measurements of a series of complexes of diphenyl pyraline hydrochloride with cobalt acetate(COAD), copper chloride (CUD), copper acetate (CUAD) and cobalt thiocyanate(COCND) as a function of temperature were undertaken. All the materials studied show semiconducting behaviour. This behaviour can be accounted for by the alternate stacking of the donor and acceptors in the crystal structures. The activation energy of the complexes range between 0.36 and 1.40 eV.

Keywords : Charge-transfer complexes, electrical conductivity, crystal structure, diphenyl pyraline hydrochloride, anti-histamine.

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Electrical phenomena associated with organic compounds has been the interest of many investigators engaged in materials research. Much progress has been made in the study of semiconducting properties of organic compounds. The extensive studies [1-3] on the electrical properties of organic materials have revealed many interesting aspects of their behaviour. The very high resistivity of organic semiconductors as compared to their inorganic counterparts is one of the interesting features. This might be attributed to the high intermolecular barrier for the conduction forces between the organic molecules. Charge transfer complexes partially overcome this difficulty. Akamatu and his associates [4] have investigated the electrical properties of aromatic hydrocarbon-halogen complexes. Since then studies on the conducting properties of a large number of charge-transfer complexes have been conducted. In crystalline materials, the electrical conductivity is confined to a particular direction resulting in large anisotropy. Many organic charge-transfer complexes exhibit conductivities ranging between $10^{-20}\,\Omega^{-1}\,\text{cm}^{-1}$ and near metallic conductivity [5].

The structural investigations of antihistamines are of great interest due to the different type of interactions involved in the constituents and their important biological activities. Diphenyl pyraline hydrochloride (DPH) is one such antihistamine, the structure of which has been reported [6]. We have reported the structure of the complex of cobalt chloride with DPH [7]. The complexes of this material with various metals have been investigated for a better understanding of their functions. We report here the resistivity measurements of complexes of DPH, viz., cobalt acetate with DPH(COAD), copper chloride with DPH(CUD), copper acetate with DPH(CUAD) and cobalt thiocyanate with DPH(COCND).

The resistance measurements of the complexes under study were carried out on pellets for COAD, CUD and CUAD and on single crystals of COCND. Keithley 195A Digital Multimeter was employed for the measurement of resistance. As the sample exhibited resistance greater than 20 $M\Omega$ at room temperature, two probes with silverised contacts were used for resistance measurements. Digital temperature controller having an accuracy of ±1% of the reading was used to set the temperature of the chamber to any desired value. The resistances of the samples were measured in the temperature range 340-500 K for every 5 K increment. Temperature was measured with Cromel-Alumel thermocouple (*K* type).

The resistance of the complexes range between 10^3-10^6 ohm. The degree of fall of resistance with temperature differs between COCND and COAD as well as between CUD and CUAD in spite of having the same metal atoms. The variation of the resistance can be explained by the expression

$$R = R_0 \exp(-E_a/kT)$$

where E_a = Activation energy, k = Boltzmann constant.

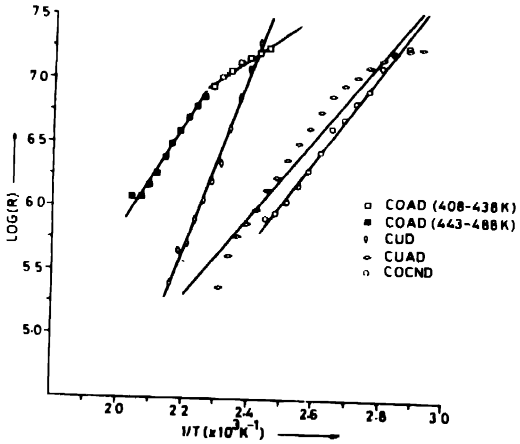

Figure 1. Log R *vs* 1/*T* plot

Table 1. Activation energies of complexes.

Complex	Slope of log(R) vs 1/T plot	Correlation coefficient	Activation energy (eV)
COAD (408-438 K)	1813.76	0.98	0.3600
COAD (443-488 K)	4186.07	0.99	0.8308
CUD	7088.02	0.99	1.4067
CUAD	3138.67	0.95	0.6229
COCND	3490.82	0.99	0.6928

The log(R) *vs* 1/*T* plots for the complexes are shown in Figure 1. The activation energies of these complexes are given in Table 1. Attempts are underway to understand the behaviour of these materials in terms of the underlying crystal structure. A typical packing of the molecules of the DPH complex with cobalt chloride is shown in Figure 2 [7]. In some cases, the stacking of the molecules in the crystal structure has favoured conduction [8] while in others it leads to a poor conductivity of the sample [9].

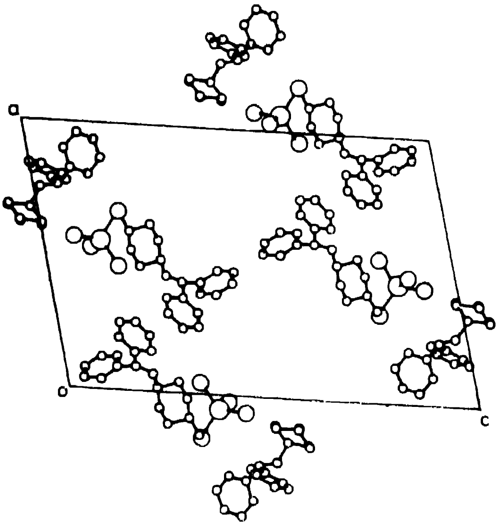

Figure 2. Packing of the molecules down b of diphenyl pyraline hydrochloride – cobalt chloride complex

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