

환경일반-5 A Study on the Environmental Hormone.

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1. ABSTRACT

To determine for the hybridization, we have investigated by UV spectroscopic method. This complex behavior as nonelectrolytes in polar aprotic solution with molar conductivities. The techniques of pulse and cyclic voltammetry have been applied to the determination of $(E_{1/2})_2 - (E_{1/2})_1$ for two-step electrochemical charge transfers. A simple amplitude has been derived for the dependence of the differential-pulse response on $(E_{1/2})_1$ and $(E_{1/2})_2$. The use of the peak-to-peak separation in cyclic voltammetry has also been evaluated. Comparison with a differential pulse and cyclic voltammetry methods shows agreement of comproportionation constant(K_c) within 50%.

2. Introduction

To our knowledge, all synthetic copper complex that exhibit reversible reductions do so in (a) a one-electron redox reaction presumably yielding a Cu(I), Cu(II) product(1) or (b) two one-electron steps with a significant potential separation presumably yield a Cu(0), Cu(I) product.(2) The net result of this process is the transfer of two electrons at the same potential. The molecular exhibiting the peculiar electrochemical properties described here is the neutral, monoclear copper(II) chelate(ligand) of bis-phenol A, $[\text{Cu}(\text{BPA})_2]$, and $[\text{Co}(\text{BPA})_2]$.

3. Results and Discussion

UV and Electronic Absorption Properties.

UV-visible spectroscopy. Between 23086.08 and 25520.94Cm^{-1} , we find the envelopes of d-d transitions($\epsilon = 0.98 \sim 1.68\text{M}^{-1}\text{Cm}^{-1}$). Accordingly, compound exhibits two bands at 23086.08 and 25520.94Cm^{-1} that can be assigned as d-d transition or charge transfer.(3) The spin state of the central metal(high-spin) depends on the relative magnitudes of crystal field splitting energy(Δ_0) and spin pairing energy(P). The magnitude of Δ_0 can be determined by investigating the energy difference between the two bands at V_1 and V_2 in the free metal ion and in its compound. On the basis of the values, the Δ_0 value for compound can be calculated as 2434.86Cm^{-1} , and its P value as 3156.30Cm^{-1} . This value indicate that the mean value is less than

the mean P value, and therefore this compound is expected to be in the high-spin state. It is well known that with increasing crystal field strength, the electrons will preferentially occupy the unstable t_{2g} orbitals.(4) The electronic structure of this compound might be predicted on the basis of electron configuration of metals. According to the calculations(Δ_0), the highest energy band might be assigned as a $d_{xy}, d_{yz}, d_{xz}(\text{nonbonding}) \rightarrow d_{x^2-y^2}$ transition that is a metal-centered d-d transition. The hybridization of this compound in the high spin state can be determined to an outer orbital((n)s(n) p_x (n) p_{y^2} (n) $d_{x^2-y^2}$).

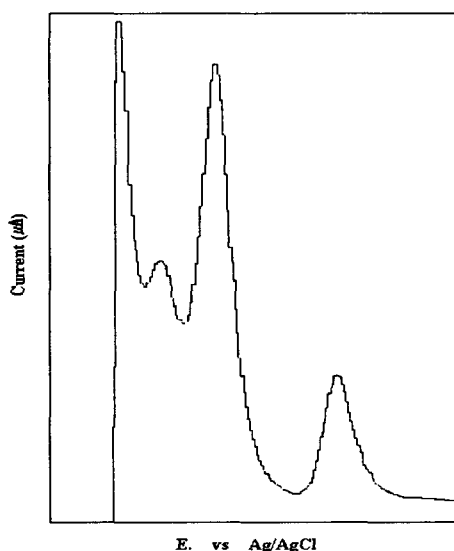


Fig.1. Current-potential curve for differential-pulse voltammetry of 1mM [Co(BPA)₂] in DMSO solvent with 0.1M TEAP at 25°C

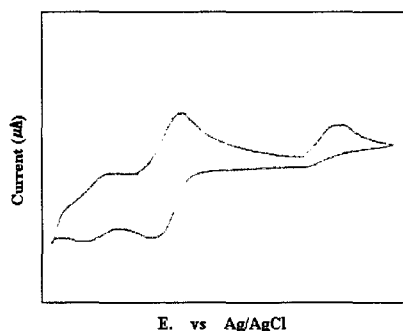


Fig.2. Cyclic voltammogram for 1mM [Co(BPA)₂] in DMSO solvent with 0.1M TEAP at 25°C

Reference

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