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Dithiocarbamate Induced Catalytic Hydrogen Wave for the determination of Iron (II) in Waters and Leafy Vegetables: Experimental and Computational Approach

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A simple, sensitive, selective and robust catalytic hydrogen wave method was developed by novel dithiocarbamates (ammonium 2,6-dimethyl morpholine dithiocarbamate and ammonium 3-methyl piperidine dithiocarbamate) using DC polarography. This method was based on the interaction of Iron(II) with dithiocarbamates in the presence of buffer (NH_4Cl-NH_4OH) at pH 6.6/6.4 to produce catalytic hydrogen currents at -1.39/-1.32V vs SCE respectively. The optimized experimental conditions were established by investigating the pH effect, supporting electrolyte (NH_4Cl-NH_4OH), and concentration of ligand. Thereafter, adverse ions effect on wave height was evaluated to enhance the selectivity of the present method. Additionally, the density functional theory calculations of ammonium 3-methyl piperidine dithiocarbamate revealed a smaller HOMO-LUMO energy gap than ammonium 2,6-dimethyl morpholine dithiocarbamates, suggesting that ammonium 3-methyl piperidine dithiocarbamates have a superior propensity to act as an electron donor to Iron(II). The reported analytical method was successfully applied for the detection of Iron (II) in different water and leafy vegetable samples with recoveries ranging from 97-99 %.

Keywords: D.C. polarography; Catalytic hydrogen currents; Iron (II); Ammonium 2,6-dimethyl morpholine dithiocarbamates; Ammonium 3-methyl piperidine dithiocarbamates; Water and Leafy vegetable samples; Density functional theory and HOMO-LUMO calculations

FULL TEXT