

# Reactivity descriptors for Cu bis-phenanthroline catalysts for the hydrogen peroxide reduction reaction

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## Abstract

Following previous studies where the metal-centered redox potentials of MN<sub>4</sub> complexes are proposed as a reactivity descriptor for different electrochemical reactions, in the present work we expand this idea to a series of substituted Cu(I)-phenanthrolines adsorbed on glassy carbon electrodes as catalysts for the hydrogen peroxide reduction reaction (HPRR) in aqueous media. As the foot of the wave for HPRR on Cu-based modified electrodes is closely related to the Cu(II)/Cu(I) formal potential, we have found a linear correlation between the catalytic activity expressed as (log i)(E) and the E-Cu(II)/Cu(I)degrees' redox potential of the complexes with a slope (dE degrees/dlogi)(E) close to +0.120 V dec(-1), showing that the catalytic activity increases with the shift of E-Cu(II)/Cu(I)degrees' to more positive potentials as a result of the electron-withdrawing nature of the substituents on the ligands. Moreover, the theoretical differences in the calculated chemical potentials (Delta mu) of the reactive species follow a similar trend with the E-Cu(II)/Cu(I)degrees' where a positive shift of this parameter is related with a higher Delta mu and in consequence, with high catalytic activity. Furthermore, this strategy can be used for the smart design of biosensors as it was shown by the electroanalytical results. (C) 2020 Elsevier Ltd. All rights reserved.

## Palabras clave

**Palabras clave de autor:** [Hydrogen peroxide reduction reaction](#); [Reactivity descriptors](#); [Copper catalysts](#); [Hydrogen peroxide sensor](#)

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