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Effect of substituent position and metal type on the electropolymerization properties of chalcone substituted metallophthalocyanines

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1.1. Materials

(2E)-3-[4-(Dimethylamino)phenyl]-1-(4-hydroxyphenyl)prop-2-en-1-one 1,¹ 4-nitrophthalonitrile 2² and 3-nitrophthalonitrile 3³ were prepared according to the literature. All reagents and solvents were of reagent grade quality and were obtained from commercial suppliers. All solvents were dried and purified as described by Perrin and Armarego.⁴

1.2. Equipment

The IR spectra were recorded on a Perkin Elmer 1600 FT-IR spectrophotometer, using KBr pellets. ¹H and ¹³C-NMR spectra were recorded on a Bruker Avance III 400 MHz spectrometers in CDCl₃ and chemical shifts were reported (δ) relative to Me₄Si as internal standard. Mass spectra were measured on a Micromass Quatro LC/ULTIMA LC–MS/MS spectrometer. MALDI-MS of complexes were obtained in dihydroxybenzoic acid as the MALDI matrix, using a nitrogen laser accumulating 50 laser shots, with a Bruker Microflex LT MALDI-TOF mass spectrometer. Optical spectra in the UV-vis region were recorded with a Perkin Elmer Lambda 25 spectrophotometer. Melting points were measured on an electrothermal apparatus and are uncorrected.

1.3. Electrochemical measurements

The cyclic voltammetry (CV) and square wave voltammetry (SWV) measurements were carried out with Gamry Interface 1000 potentiostat/galvanostat controlled by an external Pc and utilizing a three-electrode configuration at 25°C. The working electrode was a Pt disc with a surface area of 0.071 cm². A Pt wire served as the counter electrode. Saturated

calomel electrode (SCE) was employed as the reference electrode and separated from the bulk of the solution by a double bridge. Electrochemical grade TBAP in extra pure DCM was employed as the supporting electrolyte at a concentration of 0.10 mol dm⁻³.

References

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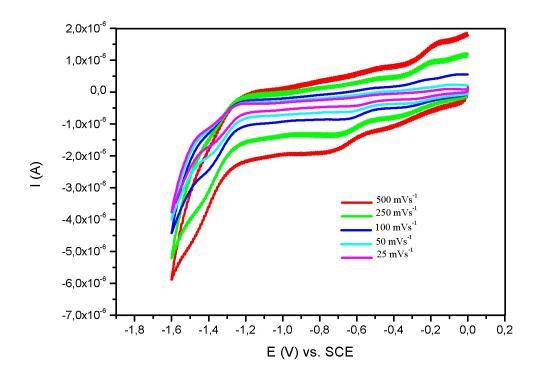


Figure S1. CVs of CoPc (6) recorded at various scan rates on a Pt working electrode in DCM/TBAP

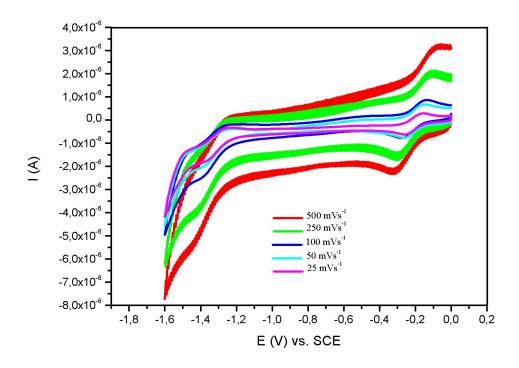


Figure S2. CVs of CoPc (7) recorded at various scan rates on a Pt working electrode in DCM/TBAP

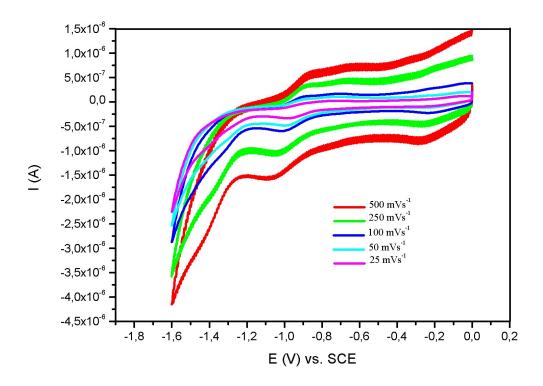


Figure S3. CVs of MnPc (8) recorded at various scan rates on a Pt working electrode in DCM/TBAP

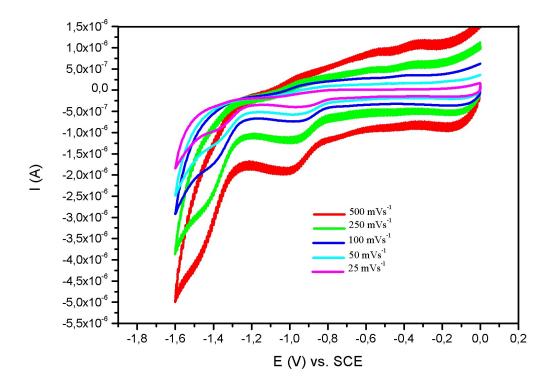


Figure S4. CVs of MnPc (9) recorded at various scan rates on a Pt working electrode in DCM/TBAP