Supplementary Material (ESI) for Analyst

Non-linear multivariate curve resolution analysis of voltammetric pH titrations

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SUPPLEMENTARY MATERIAL

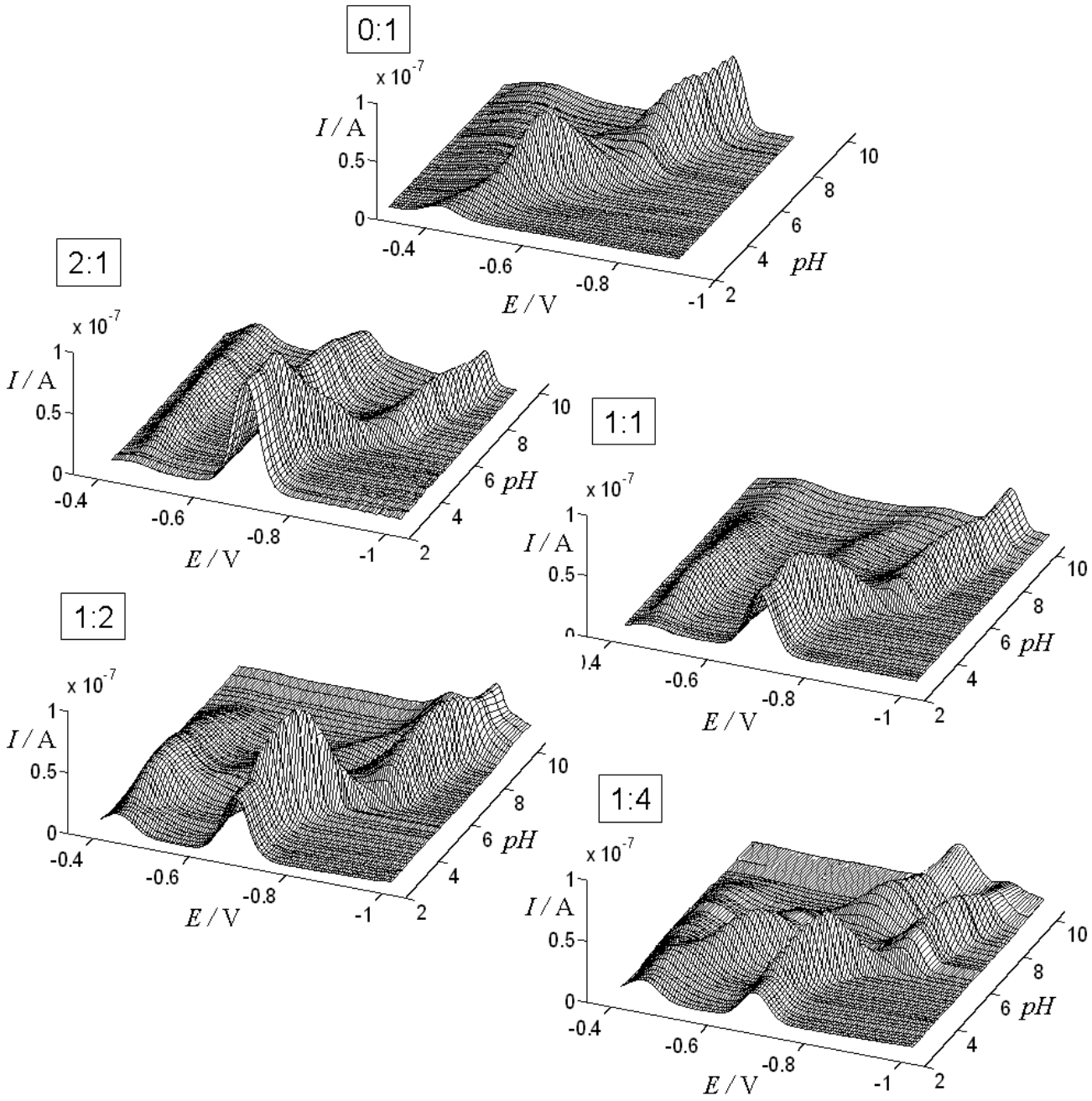

Figure I

Experimental data matrices (currents *versus* potential and pH) obtained in DPP pH titrations of the Cd(II)-PC_2 system with a KNO_3 concentration of 0.1 mol L^{-1} and at different metal-to-ligand ratios (shown inside the boxes). The total concentrations of Cd(II)/PC_2 were 0/20, 20/10, 10/10, 10/20 and 5/20 μmol L^{-1}, respectively.

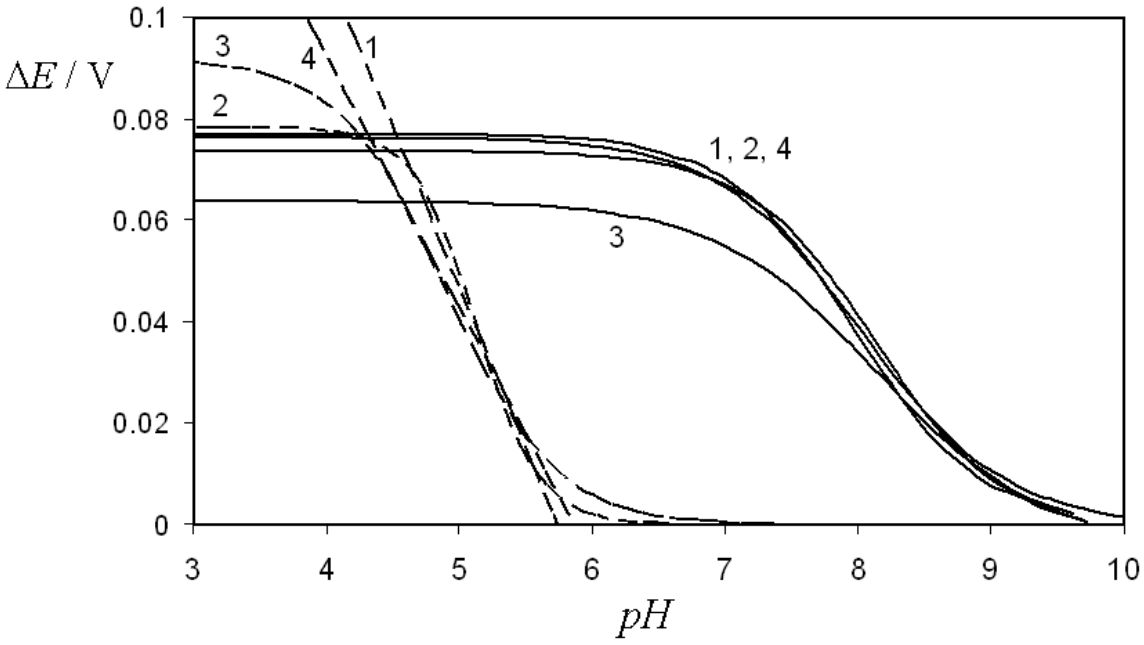

Figure II

Comparison of the fitted potential shifts as function of pH obtained by *pHfit* program from DPV measurements on the Cd(II)-PC_2 system at different metal-to-ligand ratios: 1) 2:1, 2) 1:1, 3) 1:2 and 4) 1:4. Dashed lines denote weakly bound Cd(II) whereas solid lines stand for strongly bound Cd(II).

List of files included into the programs.zip file:

peakmaker.m	Matlab program for the visual initial estimation of pure voltammograms.
pHfit.m	Matlab program for the fitting of experimental data matrices by means of potential shift correction.
shiftcalc31.m shiftcalc32.m cgolay.m genfactor.m golay.m grampoli.m negtozero.m polipes.m	set of Matlab programs which are used by peakmaker and pHfit (they have to be also in Matlab path).
tutorial.pdf	Tutorial dealing with the use of the previous programs
pHfitsample.mat	Matlab workspace containing data of the present work that can be used to practise with the programs.