Abstract

By means of electrochemical techniques, the electroreduction of polynitrocalix[4]arenes – molecules with multiple redox centers - was investigated and described. Based on interpretation of experimental data and on their correlation with quantum chemical calculations the relationship between structure and redox properties of the title molecules was revealed and discussed. It was shown that the tetranitrocalix[4]arenes involve two different couples of equivalent nitrogroups, what confirms experimentally the pinched shape of the molecule even in solution. The sequence of reduction steps was determined and the corresponding mechanism described. In the first part of the thesis different reduction mechanisms of p-substituted nitroaromates were found in dependence on substitution. It points to an important influence of lower ring substitution on the redox properties of the whole tetranitrocalix[4]arene.