

ABSTRACT

Determination of correct amount (concentration) of phytic acid is of vital importance when dealing with protonation and/or metal complexation equilibria. The main aim of the first part of the Thesis was to evaluate and develop an analytical procedure for phytic acid/phytate standardization. A novel approach for precise and reliable alkalimetric assay of phytic acid, based on the difference between end points of potentiometric titration, has been presented. Twelve phytic acid protons are classified into three groups of acidity, which enables detection of 2 to 3 distinct equivalent points depending on experimental conditions, e.g. counter-ion concentration. Using the differences between individual equivalent points enables correct phytate determination as well as determination of initial protonation degree and/or identification of contamination. Impact of uncertainty of phytate amount on the calculation of protonation constants has been evaluated using computer simulation program (Hyperquad2013). With the analysis of titration curves different binding sites on phytate ligand have been proposed for complexation of Ca(II) and Fe(III) ions.

In the second part of the Thesis the main aim was to obtain a deeper insight into the voltammetric behavior of iron(III) in the presence of phytate ligand at different pH and various ligand to molar ratios using polycrystalline gold electrode and hanging mercury drop electrode, which was used for the first time for iron(III) phytate investigation. According to cathodic and anodic processes, which are shifted towards negative direction in the presence of phytate, the diffusion-controlled reduction of Fe(III)-phytate proceeds via two predominant species depending strongly on the pH of the media. We assumed that affinity of Fe(III) for octahedral coordination induces inversion of phytate molecule from equatorial to the axial conformation, which is the reason for significantly higher stability constants and considerably negative reduction potentials. Reduction of Fe(III)-phytate proceeds via an involvement of one proton per one electron and due to the irreversibility of the process voltammetric determination of stability constants may lead to an overestimation of their values. Diffusion coefficient, charge transfer coefficient, and standard rate constant for an electron transfer were determined using HMDE, which enables good repeatability, contrary to the PGE, which exhibits “memory” effect due to adsorption of intermediates.

Keywords: Phytic acid; potentiometric standardization; calcium(II) and iron(III) phytates, cyclic voltammetry, PGE, HMDE, metal complex stability constants