

Calcium Complexing Properties of Isosaccharinate Ion in Highly Alkaline Environment

Authors : Csilla Dudás, Éva Böszörményi, Bence Kutus, István Pálinkó, Pál Sipos

Abstract : In this study the behavior of alpha-D-isosaccharinate (2-hydroxymethyl-3-deoxy-D-erythro-pentionate, ISA⁻) in alkaline medium in the presence of calcium was studied. At first the Ca-ISA system was studied by Ca-ion selective electrode (Ca-ISE) in neutral medium at T = 25 °C and I = 1 M NaCl to determine the formation constant of the CaISA⁺ monocomplex, which was found to be $\log K = 1.01 \pm 0.01$ for the reaction of $\text{Ca}^{2+} + \text{ISA}^- = \text{CaISA}^+$. In alkaline medium pH potentiometric titrations were carried out to determine the composition and stability constant of the complex(es) formed. It was found that in these systems above pH = 12.5 the predominant species is the CaISA⁺OH complex. Its formation constant was found to be $\log K = 3.04 \pm 0.05$ for the reaction of $\text{Ca}^{2+} + \text{ISA}^- + \text{H}_2\text{O} = \text{CaISA}^+\text{OH} + \text{H}^+$ at T = 25 °C and I = 1 M NaCl. Solubility measurements resulted in data consistent with those of the potentiometric titrations. Temperature dependent NMR spectra showed that the slow exchange range between the complex and the free ligand is below 5 °C. It was also showed that ISA⁻ acts as a multidentate ligand forming macrochelate Ca-complexes. The structure of the complexes was determined by using ab initio quantum chemical calculations.

Keywords : Ca-ISE potentiometry, calcium complexes, isosaccharinate ion, NMR spectroscopy, pH potentiometry

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