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Composition, stability and stereo effects of zirconium(IV) *dl*-tartrate formation

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Abstract

The system of zirconium(IV) – *dl*-tartaric acid for metal: ligand 1: 1, 1: 2 and 1: 3 ratios in aqueous solution has been studied by means of using potentiometric titration method in combination with mathematical modeling. The comparison of Bjerrum functions from pH for zirconium(IV) systems: *d*-tartaric acid and zirconium(IV): *dl*-tartaric acid, has revealed the following features in the behavior of the curves: the degree of titration for the complexes at a fixed pH value for systems with *dl*-tartaric acid is more than for *d*-acid. The CPESSP software complex has calculated the composition, stability constants and molar fractions of zirconium(IV) tartrate accumulation. It has been also found that at a ratio of 1: 1 for Zr(IV) and ligand (H_4Tart) ions in the system under study $ZrHTart^+$ is formed, which is tetramerized into $Zr_4Tart_4^0$ and, further, tetranuclear particles of varying degrees of deprotonization are formed, as well as mononuclear forms. In a strongly alkaline pH environment > 10, Bjerrum curves for *d*- and *dl*-tartaric acids overlap each other and correspond to hydroxocomplexes of varying degrees of titration. For the 1: 2 ratio, the composition of the complexes for the zirconium(IV) – *dl*-H_4T system is slightly different; compared to the zirconium(IV) – dH_4T system, differences are clearly observed for both low and high concentrations. Based on these data, a complex formation scheme in the Zr(IV) – *dl*-tartaric acid system has been proposed for all the ratios studied. The characteristics of stereoselective diastereomer formation have been calculated. It has been revealed that in the medium of racemic tartrate, *ddd*- and *lll*-$Zr(H_2Tart)_2(HTart)^{3-}$ forms, as well as $Zr(H_2Tart)(HTart)_2^{4-}$ $Zr(HTart)_3^{5-}$ are formed on a stereoselective basis.

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