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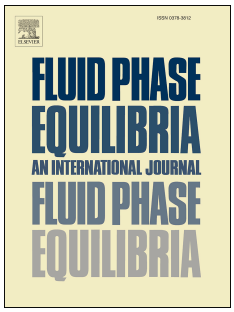

Modeling solubility and acid-base properties of some polar side chain amino acids in NaCl and $(CH_3)_4NCl$ aqueous solutions at different ionic strengths and temperatures

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ACCEPTED MANUSCRIPT

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Modeling solubility and acid-base properties of some polar side chain amino acids in NaCl and $(CH_3)_4NCl$ aqueous solutions at different ionic strengths and temperatures

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A B S T R A C T

The aim of the paper is to perform a critical analysis of the thermodynamic properties of five L-α-amino acids, namely arginine, aspartic acid, glutamic acid, glutamine and histidine. New potentiometric measurements to determine protonation constants and solubility (not for arginine) in NaCl and $(CH_3)_4NCl$ aqueous solutions are reported, in order to investigate the medium effect. A preliminary analysis of the state of art evidenced the considerable amount of data in the ionic strength range $0 < I$ / mol kg^{-1} ≤ 0.1 and a lack of data (especially for arginine and glutamine) above 0.1 mol kg^{-1}. For this reason, this paper deals with an analysis of both the literature and the new experimental data, assigning a weight to each datum as a function of its reliability. The ionic strength dependence of the protonation constants was interpreted using the EDH (Extended Debye-Hückel), the SIT (Specific ion Interaction Theory) and the Pitzer approaches. Simultaneous analysis of solubility data and protonation constants allowed us to obtain the Setschenow and the activity coefficients of all the species involved in the equilibria. The differences between the two media were also interpreted considering the formation of weak complexes between the ions of the supporting electrolytes and the ligands according to the complex formation model.

Finally, recommended, tentative or provisional data for protonation constants and protonation enthalpy changes of the five amino acids at different temperatures and ionic strengths is provided.

Keywords: Amino acids; Protonation constants; modeling; thermodynamics; weak complexes; solubility

1. Introduction

In this paper, the acid-base properties and the thermodynamic parameters (protonation constants, enthalpy change, total and specific solubility, weak complexes) of some L-α-amino acids were investigated. The ligands under study, whose structures are reported in Scheme 1, belong to the class of amino acids with polar

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