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International Conference

Thermodynamics 2007

26-28 September 2007, IFP - Rueil-Malmaison (France)

Under the auspices of

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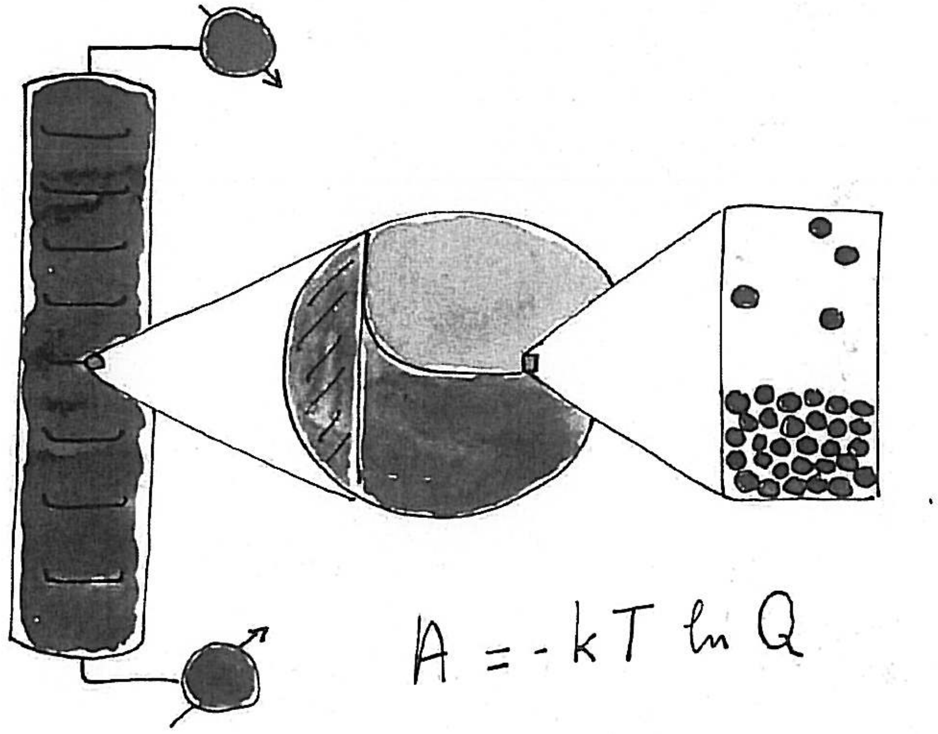
Event n°670



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Water Activity in Aqueous Amino Acid Solutions, with and without KCl, at 298.15 K

Project POCTI/40179/EQU/2001

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❖ Introduction

The study of physical chemical properties of amino acids (AA) aqueous solutions have been a very important studied subject, not only because they are the basic building blocks of proteins and peptides but also for their importance in industrial processes, particularly for pharmaceutical and food industries.

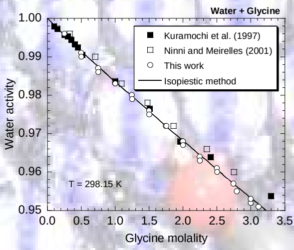
In this work an humidity sensor instrument was used to measure water activity in aqueous solutions of DL-alanine, glycine or L-serine with potassium chloride, molality ranging form 0.0 to 3.0. The reliability of the method was checked comparing the experimental data with literature values, proving to be very accurate. The calculated AA molal activity coefficients showed good consistency with those obtained using the isopiestic method, and the ternary data is very useful to extend the capabilities of thermodynamic models to higher salt and AA concentrations.

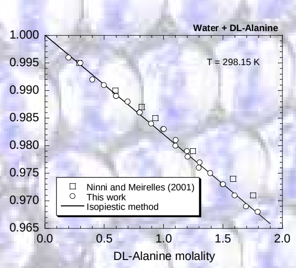
❖ Experimental Data

An humidity sensor instrument (*Lab*Master-Novasina) with a controlled chamber temperature (±0.1 K) was used to measure water activity in aqueous solutions of DL-alanine, glycine or L-serine, with potassium chloride, molality ranging from 0.0 to 3.0, at 298.15 K.

In order to attain high accuracy measurements (±0.001 aw units), a calibration curve was constructed everyday, using KCl aqueous solutions, in the appropriated electrolyte molality range.

The quality of the obtained data can be checked in the figures shown.



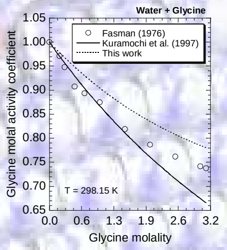


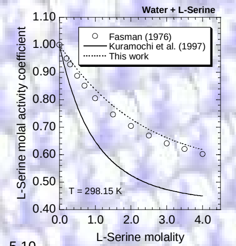
❖ Development and Discussion

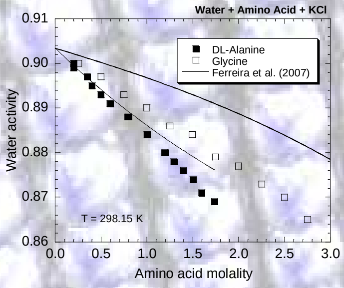
For binary systems, water activity data were correlated either by the UNIQUAC model or Pitzer-Simonson-Clegg (PSC) equations allowing the calculation of AA molal activity coefficients. As can be seen in the figures, results from this work are more consistent with the values obtained with the isopiestic method, than those found by Kuramochi et al. (1997) using vapour pressure measurements.

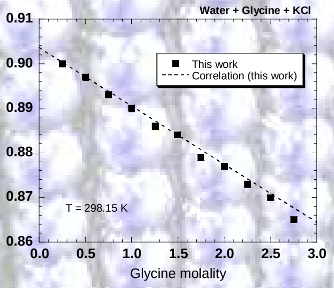
For ternary systems water-KCl with AA, Ferreira et al. (2007) showed the good capabilities of the PSC equations in their thermodynamic description. The only thermodynamic properties used to estimate the parameters representing the ternary interactions were AA solubility and KCl activity coefficients. The left side figure below shows a comparison between the measured and predicted water activities in an 3 molal aqueous KCl solution with amino acids. The results are poor.

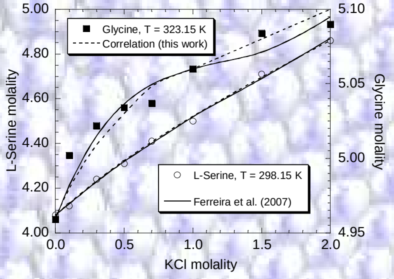
Therefore, the new experimental data was used to improve the consistency and capability of PSC equations in the representation of several properties of the aqueous AA solutions with electrolytes, namely, water activity as can be observed in the figure below (middle). A comparison for the correlation of the AA solubility, using or not the data measured in this work, is also shown below (figure on the right).











❖ Conclusions

A new simple, fast and reliable experimental procedure is proposed to measure water activity in aqueous AA solutions with or without a salt.

The proposed methodology allows the calculation of unsymmetric molal AA activity coefficients in water highly consistent with those calculated applying a virial expansion to fit osmotic coefficients measured by the isopiestic method.

Water activity measured in the ternary systems is useful to extend, consistently, the thermodynamic description of water + AA + electrolyte systems to broader salt and AA molalities.

Governo da República Portuguesa

Financiamento FCT/POCTI
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