Scientific paper

Activity of Water, Osmotic and Activity Coefficients of Sodium Glutamate and Sodium Aspartate in Aqueous Solutions at 310.15 K

Elena N. Tsurko,[1]* Roland Neueder[2] and Werner Kunz[2]

[1] *Scientific-Research Institute of Chemistry, Karasin National University, Svoboda Sq.4, 61077 Kharkiv, Ukraine*

[2] *Institute of Physical and Theoretical Chemistry, University of Regensburg, D-93040 Regensburg, Germany*

* *Corresponding author: E-mail: Jelena.N.Tsurko@univer.kharkov.ua*

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Dedicated to Professor Josef Barthel on the occasion of his 80th birthday

Abstract

The vapour pressures of aqueous solutions of sodium L-glutamate (m_i = 0.05–0.57 mol kg^{-1}) and sodium L-aspartate (m_i = 0.005–0.48 mol kg^{-1}) were precisely measured at T = 310.15 K and the activity of water and the osmotic and activity coefficients of the solutes were calculated from these data. The concentration dependence of the osmotic coefficients is described with the help of the Pitzer equation and the mean spherical approximation (MSA). It is shown that it is possible to describe thermodynamic properties of sodium aspartate and sodium glutamate solutions up to 0.5 molkg^{-1} with distance parameter R as the single fit parameter.

Keywords: Vapor pressure osmometry, osmotic coefficients, sodium L-glutamate, sodium L-aspartate, short-range interactions, electrostatic interactions

1. Introduction

The description of intermolecular interactions in amino acid and protein solutions is essential for the validation of solution theories as well as for the understanding of various effects in biophysics. The modeling is difficult, because amino acids exist as zwitterions, ions and uncharged species, which all contribute to the activity coefficients.

Some experimental thermodynamic data on amino acid and protein solutions are given in handbooks.[1,2] But there is still a need for more data in order to enlarge the basis for appropriate modeling of biosystems.[3,4]

Activity coefficients in aqueous electrolyte-amino acid mixtures have been measured in some studies[5–8] and the results have been explained with the help of an adequate mean force potential between dipolar and normal ions.[9,10]

In our previous studies we have measured the activity of water and osmotic coefficients in glycine, L-histidine, glutamic acid, their salts and Boc-derivatives.[11,12] In the present work we are further concentrating on the properties of the salts of two biologically important three-basic amino acids: sodium aspartate (NaAsp) and sodium glutamate (NaGlu).

Thermodynamic data on NaGlu and NaAsp aqueous solutions are useful e.g. for the modeling of the influence of the ion channels on the signal transmission in a human body cell (e.g. polyglutamate model of ion channels).[13,14]

Solubility data for L-asparagine in water and in aqueous solutions for glycine, diglycine, lysylglutamic acid, alanine and dl-α-aminobutyric acid are presented in the work of Cohn et al.[15] and revealed that there is a considerable complexity in the calculation of activity coefficients of L-asparagine. Density data of L-aspartic and L-glutamic acid in aqueous solutions at 288.15–318.15 K and the analysis of apparent molar volumes are provided in a recent paper by Banipal et al.[16] who discussed the results with the help of interparticle hydrophobic interactions de-

pending on the length of the alkyl chain and organic salt addition. The analysis of pair interaction coefficients from calorimetric data[17] for nucleic bases (Ura, Cyt, Thy, Ade) with the amino acids asparagine, glutamine, aspartic and glutamic acids shows the predominance of specific (short-range) interactions in the systems Cyt + L-Asp, Thy + L-Asp, Ade + L-Asp, Ade + L-Glu. This is due to acid-base interaction between the zwitterionic carboxylic group of amino acids and the nitrogen or oxygen atoms of nucleic bases. This tendency to association is especially pronounced for L-aspartic acid in the case of interaction with nucleic bases because of the short hydrocarbon chain. For other amino acids the association is hindered because of electrostatic interactions between NH_3^+- and COO^-- amino acid groups. The tendency to association due to acid-base interactions decreases in the order: L-Asp > L-Glu > L-Asn > L-Gln.

Osmotic and activity coefficients of some aliphatic and non-polar amino acids can be found in the literature,[18] but no data are available for aspartic and glutamic acids. The investigation of sodium aspartate and sodium glutamate is relevant for the study of the effect of increasing length and complexity of the aliphatic carbon chain[19] as well as for the charge character of the amino acid. Osmotic and activity coefficients of NaGlu from vapor pressure measurements at 298.15 K are presented in our previous work,[11] which agree with the data of Bonner[20] and deviate slightly from these of Rohdewald.[21]

Elcock et al.[22] provide conformational molecular dynamics simulations of a lysine glutamate salt bridge. Protein stabilizations are investigated at different temperatures (25, 50, 75 and 100 °C). The results demonstrate that salt bridge interactions are insensitive to temperature changes and, as such, are uniquely suited to promoting protein stability at high temperatures.

In addition to investigations at room temperature there is further interest in thermodynamic data at the temperature of the human body.[23] Therefore, in the present work, the chemical potentials of aqueous sodium L-glutamate (m_i = 0.005–0.45 mol kg^{-1}) and sodium L-aspartate (m_i = 0.005–0.4 mol kg^{-1}) are obtained from vapor pressure osmometry measurements that were performed at T = 310.15 K.

2. Experimental

2. 1. Materials and Reagents

L-glutamic acid monosodium salt hydrate (Sigma, 99–100%), L-aspartic acid monosodium salt monohydrate (Fluka, puriss, ≥ 99%) were used without further purification. All solutions were prepared by weighing with an accuracy of 0.0001 g. Water from the millipore purification system, with a specific conductivity of 5.6×10^{-8} S cm^{-1} (25 °C), was used for the preparation of the solutions which were stored under purified nitrogen.

2. 2. Vapor Pressure Measurements

The vapor pressure osmometry (VPO) measurements were performed with a Knauer Osmomat (K-7000) that permits precise investigations down to a concentration of m = 0.005 mol kg^{-1}. With this method, the vapor pressure is determined indirectly by using thermistors to measure voltage changes caused by changes in temperature. The measuring chamber contains a reservoir of solvent and paper wicks to provide a saturated solvent atmosphere. Initially a drop of pure solvent is attached to each thermistor with the help of a syringe and after 5 minutes of equilibration the reading was adjusted to zero. Then the pure solvent on one thermistor was replaced by the solution under investigation and condensation of solvent from the vapor phase into the solution at the thermistor took place. Due to the heat of condensation the thermistor temperature rises and the vapor pressure increases. Condensation continues until the vapor pressure of the solution equals the vapor pressure of the pure solvent. Special care is taken to keep the drop size and shape equal on both thermistors.

A comparison between results obtained with this equipment and those from direct vapor pressure lowering with a classical equipment[24] has been done elsewhere[25] and shows good agreement between both techniques.

The instrument was calibrated at 310.15 K using aqueous sodium chloride solutions in the concentration range from 0.009–1.5 mol kg^{-1}, yielding a function, which correlates the panel readings to the corresponding concentrations of the sodium chloride solution. Then the measurements for the different amino acid salt solutions were carried out. For each solution 6–9 determinations (one set comprises 3 determinations and a zero point adjustment) were performed and the mean value was calculated.

3. Results and Discussion

3. 1. Activity of Water and Osmotic Coefficient

The osmotic coefficient is defined as

$$\phi = -\frac{\ln a_w}{\nu\, m\, M_w} \tag{1}$$

where a_W is the water activity, M_W is the molar mass of water, m is the solute molality and ν is its stoichiometric coefficient.

The osmotic coefficients, ϕ, of the amino acids (sodium glutamate or sodium aspartate; index: *AA*) solutions of concentration m(*AA*) were calculated from the panel reading of the osmometer and the correlation function from the calibration. This correlation function yields the concentration of the sodium chloride m(NaCl) solution,

that equals the same solvent activity as the amino acid solution. Using Eq. (2) for the two solutions (the amino acid solution and sodium chloride calibration solution) with equal solvent activity leads to the following relationship between the osmotic coefficient of the sodium glutamate (sodium aspartate) solution and that of the calibration solution

$$\phi(AA) = \frac{\nu(NaCl)\, m(NaCl)\, \phi(NaCl)}{\nu(AA)\, m(AA)} \quad (2)$$

The required osmotic coefficients ϕ(NaCl) were calculated from the respective concentration m(NaCl) with the help of the equation set developed by Gibbard and Scatchard,[26] see Appendix 1. The stoichiometric coefficients ν(NaCl) and ν(AA) were set equal to 2. From the osmotic coefficient ϕ the activity of water a_W can be obtained according to

$$\ln a_W = -2\, m\, M_W\, \phi \quad (3)$$

The experimental osmotic coefficients of NaGlu and NaAsp aqueous solutions at T = 310.15 K are presented in Table 1 and Fig.1.

Table 1. Osmotic Coefficients of Sodium Glutamate, Sodium Aspartate Aqueous Solutions, T= 310.15.

NaGlu		NaAsp	
m_i (mol kg^{-1})	ϕ	m_i (mol kg^{-1})	ϕ
0.0521	0.964	0.0498	0.970
0.0943	0.967	0.0976	0.958
0.1655	0.944	0.1558	0.946
0.2413	0.939	0.2463	0.938
0.3525	0.933	0.2925	0.931
0.3727	0.935	0.2547	0.937
0.5646	0.938	0.4823	0.919

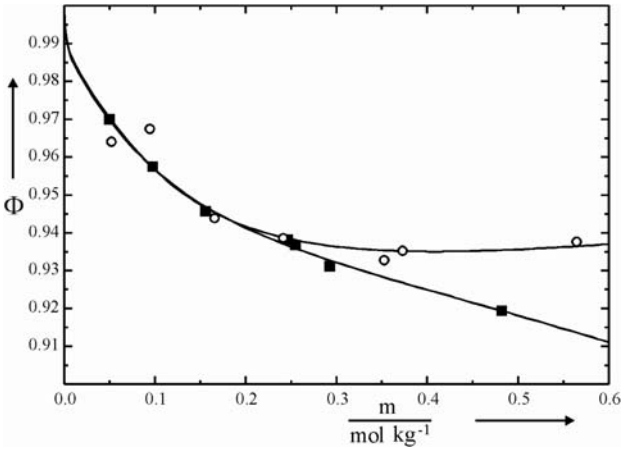


Figure 1. Osmotic coefficients of sodium glutamate (○) and of sodium aspartate (■) at 310.15 K (lines calculated with Pitzer equation)

3.2. Pitzer Equation. Mean Ionic Activity Coefficient

The mean ionic activity coefficient is calculated from the Gibbs-Duhem equation that yields a relationship between the solvent activity and the mean ionic activity coefficient $\gamma_\pm$. The definition of the osmotic coefficient leads to:

$$\ln \gamma_\pm = (\phi - 1) - \int_0^{m} \frac{(1-\phi)}{m}\, dm \quad (4)$$

Osmotic coefficients ϕ and mean molal activity coefficient $\gamma_\pm$ can be advantageously reproduced over large concentration ranges with the help of the Pitzer equations which for 1–1 electrolytes take the form[29]

$$\phi = 1 - \frac{|z_+ z_-|\, A_\phi I^{1/2}}{1 + bI^{1/2}} + mB^\phi + m^2 C^\phi \quad (5)$$

$$B^\phi = \beta^{(0)} + \beta^{(1)} \exp\left[-\alpha_1 I^{1/2}\right] + \beta^{(2)} \exp\left[-\alpha_2 I^{1/2}\right] \quad (6)$$

$$A_\phi = \frac{\sqrt{2\pi N_A d_s^*}}{3} \left(\frac{e_\circ^2}{4\pi\varepsilon_\circ \varepsilon kT}\right)^{3/2} \quad (7)$$

$$I = \frac{1}{2} \sum m_i z_i^2 \quad (8)$$

Integrating the osmotic coefficient from zero concentration to the final solute concentration m according to (4) yields the mean ion activity:

$$\ln \gamma_\pm = -\frac{|z_+ z_-|\, A_\phi I^{1/2}}{1 + bI^{1/2}} - \frac{2\,|z_+ z_-|\, A_\phi}{b} \ln\left(1 + bI^{1/2}\right) + mB^\gamma + \frac{3}{2} m^2 C^\phi \quad (9)$$

$$B^\gamma = 2\beta^{(0)} + \xi^{(1)} + \xi^{(2)} \quad (10)$$

$$\xi^{(i)} = \left(\frac{2\beta^{(i)}}{\alpha_i^2 I}\right)\left[1 - (1 + \alpha_i I^{1/2} - \frac{1}{2}\alpha_i^2 I)\exp(-\alpha_i I^{1/2})\right] \quad (11)$$

In Eqs. (5–11) I is the ionic strength, m_j is the molality of the ion of type j and z_j its valency. N_A is the Avogadro constant, k is Boltzmann's constant, e_0 is the elementary charge and ε_0 is the permittivity of vacuum. The other symbols have their usual meaning. A_ϕ is the Debye-Hückel constant for the osmotic coefficient in the molal concentration scale and can be calculated with the help of density d_s^*[27]

Table 2. Parameters of Pitzer Equation (5) for Sodium Salt Solutions (b = 1.2, α_1 = 1.4, α_2 = 10.0), T = 310.15 K

Solute	m_{max}	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	C^{Φ}	σ
NaGlu	0.57	0.03400	0.37437	4.95541	0	0.006
NaAsp	0.48	–0.09519	0.62974	4.13743	0	0.001

and relative permittivity ε[28] of pure water: A_ϕ = 0.400 kg$^{1/2}$mol$^{-1/2}$ (310.15 K). The parameters $\beta^{(0)}$, $\beta^{(1)}$, $\beta^{(2)}$, C^ϕ are Pitzer's ion-interaction parameters while α_1, α_2 and b are adjustable parameters (usually fixed to certain values). The parameters b = 1.2 kg$^{1/2}$ mol$^{-1/2}$ and α_1 = 1.4 kg$^{1/2}$ mol$^{-1/2}$ were set according to Pitzer[29,30]. Best fitting results were obtained for α_2 = 10.0 kg$^{1/2}$ mol$^{-1/2}$. As the concentration is limited to a moderate range (less than 0.6 mol kg^{-1}) the C^ϕ – parameter is set to zero as was done for NaGlu at 298.15 K[11]. The parameters $\beta^{(0)}$, $\beta^{(1)}$ and $\beta^{(2)}$ from the fitting of the experimental data are presented in Table 2.

Osmotic coefficients of sodium glutamate and sodium aspartate decrease with salt concentration. In contrast to the results for sodium glutamate at 298.15 K in our previous work[11] and in the paper of Das[31], the Pitzer-model without $\beta^{(2)}$ value is not sufficient to describe the osmotic coefficients of sodium aspartate and sodium glutamate at 310.15 K properly. According to Phutela and Pitzer[32] the $\beta^{(2)}$ contribution increases with increasing temperature. Therefore the use of an additional term ($\beta^{(2)}$) is reasonable for the second virial coefficient of Eq. (5).

To take into account all existing species (zwitterions, ions and uncharged molecules) in dilute solutions would make the data analysis much more complicated. But in the given concentration range and with the experimental uncertainties there is no need for such a complete treatment.

Table 2 shows, that the values of $\beta^{(0)}$ and $\beta^{(1)}$ are larger for sodium aspartate than for sodium glutamate, i.e. interparticle interactions are more pronounced for the amino acid anion with the shorter hydrocarbon chains. In glutamate the NH_3^+ and COO^- groups are more closely located because of the flexibility of the hydrocarbon chain and may lead to stronger electrostatic interaction. It seems, that aspartate shows a larger tendency for the association with other molecules, while glutamate is more prone to intramolecular interaction. This is in agreement with the results of the interaction study of L-aspartic acid and L-glutamic acid with nucleic bases of Kulikov.[17]

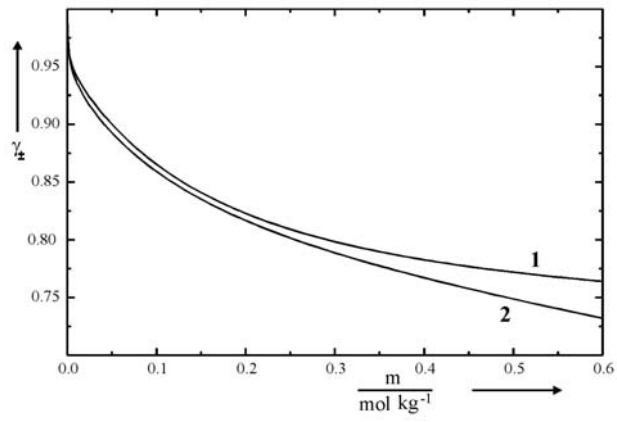
The inclusion of $\beta^{(1)}$ and $\beta^{(2)}$ in the fitting procedure is probably necessary due to hydrophobic interactions of the amino acid anions. According to Scheraga:[33] "Hydrophobic interactions are solvent induced interactions, i.e. indirect interactions among solutes, caused by the presence and the particular nature of the solvent". They are stipulated by entropy and heat-capacity increase due to "specific changes in the structure of water in the vicinity of the nonpolar molecules".

Mean ionic activity coefficients were calculated with the help of Eqs. (9–11) and the parameters from Tables 2 and are presented in Table 3. Activity coefficients decrease with concentration as can be seen in Fig. 2. Sodium aspartate shows more pronounced deviation from ideality than sodium glutamate. This is in agreement with the fact that anions with smaller hydrocarbon chains show a stronger tendency to interparticle interactions. On the contrary, glutamate has a zwitterionic structure and shows a cyclical, hydrogen-bonded structure.[20]

Finally, it should be stressed that our activity coefficients for NaGlu at 310.15 K are in good agreement with those at 298.15 K.[11,20,31]

Table 3. Mean Ionic Activity Coefficients, $\gamma_\pm$, for Sodium Salt Solutions, T=310.15 K.

m (mol kg^{-1})	NaGlu	NaAsp
0.01	0.942	0.937
0.02	0.929	0.922
0.03	0.918	0.911
0.04	0.909	0.901
0.05	0.900	0.893
0.10	0.865	0.859
0.15	0.841	0.835
0.20	0.823	0.817
0.25	0.809	0.802
0.30	0.798	0.789
0.35	0.790	0.777
0.40	0.783	0.767
0.45	0.777	0.758
0.50	0.772	0.749
0.55	0.768	0.740
0.60	0.764	0.732



Figire 2. Mean ionic activity coefficients of sodium glutamate (1) and sodium aspartate (2) at 310.15 K (calculated with Pitzer equation).

3.3. Modeling the Osmotic Coefficients of NaGlu, NaAsp with the Mean Spherical Approximation

In contrast to Pitzer's equations, the MSA is a theoretically well-based model that also allows the thermodynamic description of electrolyte solutions up to relatively high salt concentrations.[34] The osmotic coefficients of NaGlu, NaAsp were calculated with the help of the following equation:[35,36,34]

$$\phi = \frac{1+\eta+\eta^2-\eta^3}{(1-\eta)^3} - \frac{\left(\sqrt{1+2\kappa R}-1\right)^3}{24\pi\rho R^3} \qquad (12)$$

The first term of Eq. (12) is the hard sphere term with

$$\eta = \frac{\pi}{6}(\rho_+ + \rho_-)R^3 = \frac{\pi}{6}\rho R^3, \qquad \rho = (\nu_+ + \nu_-)cN_A = \nu cN_A \qquad (13)$$

with ρ_i as the particle density of species *i* and *R* the distance parameter (average diameter of the species).

The second term in Eq. (12) is the electrostatic interaction term with the MSA screening parameter $\kappa^2 = 16\pi q N_A c$ and the Bjerrum parameter $q = z_i^2 e^2/8\pi\varepsilon\varepsilon_0 kT$. A value of 74.83 has been used in the calculations for the dielectric constant of water.

In our previous paper[11] we used a third term, $(1-\alpha)/2$, in Eq.(12) that takes into account the partial dissociation via the degree of dissociation α. This term is neglected in this study, because its contribution to the final value of the osmotic coefficient is very small and does not exceed 0.002–0.005 for NaGlu and NaAsp.

The reference distance parameters *R* were assumed to be $R = r_{Glu^-} + r_{Na^+}$ for sodium glutamate, $R = r_{Asp^-} + r_{Na^+}$ for sodium aspartate. The radius of the ion $r_{Na^+} = 0.098$ nm is taken from Ref.[37,38]. The radii of the amino acids $r_{Glu^-} = 0.274$ nm, $r_{Asp^-} = 0.260$ nm were calculated from the respective molar volumes[39] according to $r = (3v/4\pi)^{1/3}$.

In the MSA analysis the *R* value is taken as an adjustable parameter. Table 4 shows the results together with distance parameters from the literature. In Fig. 3 and in Table 5 the experimental data are compared with the results of the MSA model. It can be seen that with only one adjustable parameter (distance parameter *R*) it is possible to describe osmotic coefficients of sodium aspartate and sodium glutamate up to a concentration of 0.5 mol kg^{-1} within the experimental uncertainty, which never exceeds 0.02 in all measurements.

In the range of high concentrations we found a satisfactory agreement of the experimental and the calculated data for sodium glutamate and sodium aspartate. The va-

Table 4. Comparison of MSA Distance Parameters with Literature Values.

	$R_{liter.}$(A)	$R_{fit.}$(A)	St.dev.
NaGlu	3.72	3.7	0.018
NaAsp	3.58	3.7	0.016*

* – the last point is omitted

Table 5. Comparison of the Experimental and Theoretical Osmotic Coefficient Values of Sodium Glutamate, Sodium Aspartate Aqueous Solutions at 310.15 K.

NaGlu			
m **(mol kg^{-1})**	ϕ^{exp}	***m*** **(mol kg^{-1})**	ϕ^{MSA}
0.0521	0.964	0.06	0.941
0.0943	0.967	0.11	0.933
0.1655	0.944	0.16	0.930
0.2413	0.939	0.26	0.931
0.3525	0.933	0.36	0.936
0.3727	0.935	0.41	0.940
0.5646	0.938	0.56	0.954
		R_{fit} = 3.7 A	
NaAsp			
m **(mol kg^{-1})**	ϕ^{exp}	***m*** **(mol kg^{-1})**	ϕ^{MSA}
0.0498	0.970	0.05	0.944
0.0976	0.958	0.10	0.934
0.1558	0.946	0.15	0.930
0.2463	0.938	0.25	0.930
0.2547	0.937	0.25	0.930
0.2925	0.931	0.3	0.932
0.4823	0.919	0.5	0.946
		R_{fit} = 3.7 A	

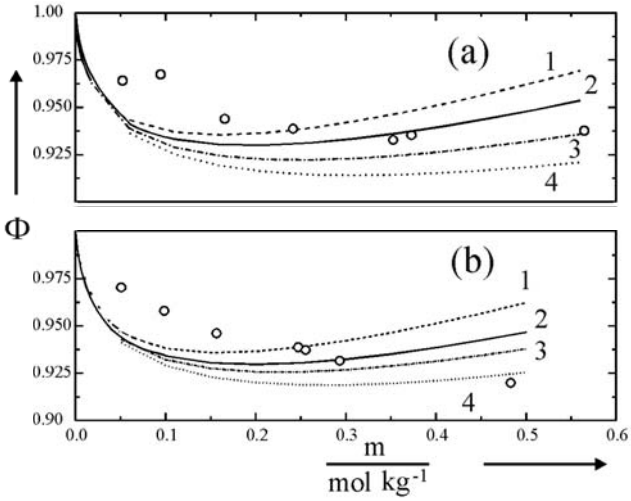


Figure 3 Osmotic coefficients of sodium glutamate (a) and of sodium aspartate (b) at 310.15 K calculated with the help of MSA equations Distance parameter for sodium glutamate: *R* = 3.9 A (1), *R* = 3.7 A (2), *R* = 3.5 A (3), *R* = 3.3 A (4) and for sodium aspartate: *R* = 3.9 A (1), *R* = 3.7 A (2), *R* = 3.58 A (3), *R* = 3.4 A (4).

lues of the adjustable parameter *R* are equal for the sodium glutamate and higher for the sodium aspartate in comparison to the sum of the ionic crystallographic radii.

4. Conclusions

In the present paper the osmotic and activity coefficients of aqueous sodium aspartate and sodium glutamate solutions were precisely determined at the temperature of the human body. The data could be described by Pitzer's equation and satisfactorily modeled with the Mean Spherical Approximation.

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Povzetek

Izmerili smo parne tlake vodnih raztopin natrijevega L-glutamata (m_i = 0.05–0.57 mol kg^{-1}) ter natrijevega L-aspartata (m_i = 0.005–0.48 mol kg^{-1}) pri 310.15 K ter izračunali aktivnost vode ter osmozne ter aktivnostne koeficiente topljencev. Koncentracijsko odvisnost osmoznih koeficientov smo opisali s Pitzerjevo enačbo ter »mean sphere approximation« (MSA). Pokazali smo, da je termodinamske lastnosti vodnih raztopin natrijevega L-glutamata ter natrijevega L-aspartata vse do koncentracije 0.5 mol kg^{-1} možno opisati s prilagajanjem le enega parametra – parametra razdalje R.

Apendix 1

Equation set for the calculation of the osmotic coefficient ϕ of aqueous sodium chloride solutions of concentration m (molkg^{-1}) as developed by Gibbard and Scatchard[26].

$$\phi = 1 - \frac{SZ}{a} + \sum_{j=1}^{w} D_j m^j \tag{1.1}$$

$$S = 1.17284 - \frac{6202.357\tau}{T_S^2\left(1+\frac{\tau}{T_S}\right)} + 54.4251\ln\left(1+\frac{\tau}{T_S}\right) - 0.161993\tau + 8.59609\cdot 10^{-5}\left(2T_S\tau+\tau^2\right) \tag{1.2}$$

$$\text{where } Z = \frac{1+X-\frac{1}{1+X}-2\ln(1+X)}{X^2};\ \tau = T - T_S;\ X = a\sqrt{m};\ T_S = 298.15K;\ a = 1.5.$$

The coefficients D_j of the power series in m of Eq. (1.1) are given by:

$$D_j = D_j^{(S)} - 0.2516103\sum_{k=0}^{w}\frac{D_j^{(k)}}{k!}\int_0^{\tau}\frac{t^k}{(t+T_S)}dt \tag{1.3}$$

with coefficients $D_j^{(S)}$ and $D_j^{(k)}$ given in the paper of Gibbard and Scatchard[26].