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Vapor−Liquid Equilibria in the System $NH_3 + H_2O$ + LiBr. 2. Data Correlation

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A quasi-chemical reaction model has been developed to correlate vapor−liquid equilibrium data for the system ammonia (NH_3) + water (H_2O) + lithium bromide (LiBr) in the temperature range from 303.15 to 473.15 K and at pressures up to 2.0 MPa. This model assumes the formation of ion clusters, i.e., Li^+ and Br^- ions surrounded by ammonia and water molecules. Further, ammonia and water molecules are assumed to form a second species of complexes. The activities of the various components in the liquid phase are modeled by the NRTL equation. The vapor phase, assumed to consist of ammonia and water only, is modeled by the equation of state of Ishikawa, Chung, and Lu.

Introduction

The systems ammonia + water ($NH_3 + H_2O$) and water + lithium bromide (H_2O + LiBr) provide two working pairs most often used today in air-conditioning systems and systems for reusing industrial waste heat, such as absorption heat pumps and heat transformers (*1*). However, these binaries have certain disadvantages which imply limitations for the working range. The use of mixtures of lithium bromide and water is limited by crystallization and corrosion occurring at high temperatures and salt concentrations. The main disadvantages of the ammonia + water system are high vapor pressures at elevated temperatures and the high content of water in the vapor phase. Considering technical applications, the last circumstance implies the use of a dephlegmator for purification of ammonia in the vapor phase. In order to overcome these difficulties, several additives have been given to ammonia + water solutions (*2*−*9*). In 1921 Foote (*2*) investigated the vapor pressure above liquid mixtures of ammonia, water, and ammonium thiocyanate. In the same year Davis, Olmstead, and Lundstrum (*3*) measured vapor pressures of the system ammonia + water + lithium nitrate. Particular solutions of the systems $NH_3 + H_2O$ with the additives $Ca(NO_3)_2$, NaI, $CaCl_2$, NH_4NO_3, and NH_4CNS were examined by David, Olmstead, and Lundstrum (*4*) also. Other ternary mixtures of known working pairs used in sorption processes are ammonia + water + sodium hydroxide (*8*) and ammonia + water + methanol (*6*). The system ammonia + water + lithium bromide has been most studied. Vapor−liquid equilibria were measured by Radermacher (*5*), Zimmermann (*7*), and Peters (*9*). Several researchers reported the density and viscosity of the liquid solutions (*10*), crystallization (*11*), and mass diffusion (*12*).

In a previous paper we reported the measurements of vapor−liquid equilibria in the system ammonia + water + lithium bromide and its industrial application. Considering the system $NH_3 + H_2O$ + LiBr as an alternative working fluid to $NH_3 + H_2O$, it is necessary to provide a model to correlate the vapor-liquid equilibria in wide temperature and pressure ranges.

In this paper we introduce a thermodynamic model which includes two quasichemical reactions to correlate the vapor−liquid equilibrium data base given by Peters et al. (**9**). After describing the so-called mixed-solvent solvation model, we give a detailed comparison between calculated and measured values of the pressure and the vapor compositions with the vapor phase.

Theoretical Model

Vapor−Liquid Equilibrium. In this section we formulate the basic equations of a thermodynamic model to calculate vapor−liquid equilibria (VLE) in the system ammonia + water + lithium bromide. We start by denoting the conditions for VLE in a system containing an aribitrary number of components i = 1, ..., N:

$$\varphi_i y_i p = \gamma_i x_i \varphi \mathrm{p}_{\mathrm{o}i} \exp[\int_{p_{\mathrm{o}i}}^{p} (v_{\mathrm{o}i}/RT)\,\mathrm{d}p] \qquad (1)$$

All symbols have their usual meaning (*13*) and are defined in the list of symbols. Aiming at a (T, x) → (p, y) type calculation (BUBL *P* calculation (*13*)) we have to determine all quantities on the right hand side of eq 1. In the next sections we give an equation of state to describe the real behavior of the gas phase and a quasi-chemical reaction model for the real liquid phase.

Equation of State. The vapor phase is assumed to consist of ammonia and water only, i.e., to include neither lithium bromide nor ionic complexes possibly being formed by Li^+, Br^-, ammonia, and water molecules, in the range of temperature 288−503 K considered. Information about the equilibium ratio of salt in the liquid and the gas phases have been given by Kuske and Stephan (*14*).

To describe the vapor phase in the investigated temperature range 288−503 K and pressure range 0.1−17 MPa, we used the equation of state (EOS) of Ishikawa (*15*)

$$Z = \frac{pV}{RT} = \frac{2V + b}{2V - b} - \frac{a}{RT^{1.5}(V + b)} \qquad (2)$$

with parameters determined for the system ammonia + water by Iseli (*16*). Here V is the molar volume and Z is the compressibility factor. For pure substances the two adjustable parameters a and b are functions of the absolute temperature. For the mixture there is an additional dependence of the parameters a_{ik} and b_{ik} ($i = k = 1$, H_2O; $i = k = 4$, NH_3) on the number of moles of each component described by Iseli. Details about the calculation of the fugacity coefficients φ_i and φ_{io} from the EOS in eq 2 are given by Peters (*9*).

Vapor Pressure and Molar Volume of Pure Substances. The vapor pressure p_{oi} and the molar volume V_{oi}

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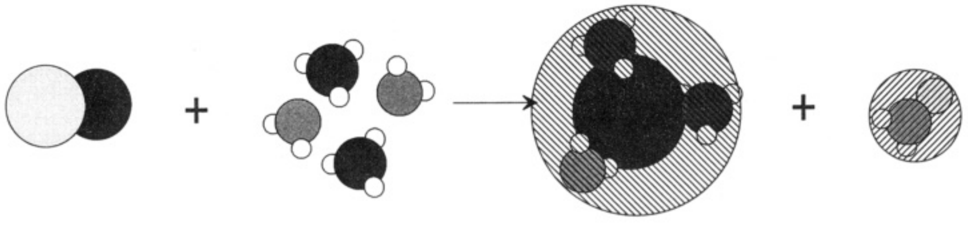

Figure 1. Example of a formation reaction of ionic clusters from LiBr, NH_3, and H_2O molecules.

of the liquid phase in the boiling state of pure component $i = 1$ or 4 can be calculated by the EOS of Garnjost (*17*) for ammonia and the EOS of Wagner of Saul (*18*) for water. In order to calculate the vapor pressure and the molar volume of ammonia at temperatures higher than the critical temperature of the pure substance, we introduced hypothetical boiling states given by eqs 3 and 4. For the vapor pressure of pure ammonia at temperatures higher than 405.5 K we employed a linear relationship

$$p^{s}_{NH_3}(T > T_{c,NH_3}) = p^{c}_{NH_3} + (\partial p/\partial T)_{c,NH_3}(T - T_{c,NH_3}) \quad (3)$$

Likewise for the molar volume at temperatures higher than $T^* = 373$ K

$$V^{s}_{NH_3}(T > T^*) = V_{NH_3}(T^*) + (\partial V/\partial T)_{T^*}(T - T^*) \quad (4)$$

Solvation Model. The basic idea underlying the model is that LiBr after dissolving in the solution is partly dissociated. The ions Li^+ and Br^- generated in this way immediately are coated with ammonia and water molecules, forming ionic clusters which can be considered as new components in the sense of equilibrium thermodynamics. The quasi-chemical equilibrium established in this way in the liquid phase can be described by the stoichiometric equation

$$mH_2O + nNH_3 + LiBr \rightleftharpoons K^+ + A^- \quad (5)$$

$$K^+ = Li^+(H_2O)_{m^-}(NH_3)_{n^-} \quad (6)$$

$$A^- = Br^-(H_2O)_{m^-}(NH_3)_{n^-} \quad (7)$$

To give an example, the formation of ionic clusters is sketched in Figure 1. The parameters m, n, $m^{\pm}$, and $n^{\pm} \geq 0$ are so-called solvation numbers of the reaction in eq 5. They are related by

$$m = m^+ + m^- \quad (8)$$

$$n = n^+ + n^- \quad (9)$$

$$k^+ = m^+ + n^+ \quad (10)$$

$$k^- = m^- + n^- \quad (11)$$

The solvation number m has been discussed for a reaction similar to eq 5 in the system H_2O + LiBr by Peters and Keller (*19*):

$$mH_2O + LiBr \rightleftharpoons Li^+(H_2O)_{m^-} + Br^-(H_2O)_{m^-} \quad (12)$$

The solvation number m included in this equation originally has been considered to be a constant (*20*). However, there is physicochemical evidence that m strongly depends on the concentration $x°_{LiBr}$ of LiBr originally, i.e., prior to ionization, being attained in the solution (*21*). Therefore, we have considered m to be a function of this quantity.

Table 1. Number of Water Molecules in the First Hydration Shell at Infinite Dilution Given by Marcus

method	m^+	m^-
X-ray studies	4	6
Monte Carlo studies	6	
corrected Stoke's radii	7.4	3.4
from $\Delta S°_{hydr}$	4.3	(<0)
from ${}^{\phi}K^{\infty}$	2.9	0.8
from $\gamma_{\pm}$	3.4	0.9

Table 2. Numerical Values of Parameters in the Solvation Numbers Model, Eqs 14–19

a_o^+	a_o^-	$\hat{a}$	a_e^+/(J mol^{-1})	a_e^-/(J mol^{-1})
0.1212	1	1	291	14 375

Interpolating numerical values of m gained by optimization procedures in fitting analytic and experimental VLE data over wide ranges of temperature and concentration, we found the relation

$$m = 4 - 5x°_{LiBr} \quad (13)$$

indicating that m decreases with increasing initial salt concentration. Marcus (*22*) reported several determination methods of the solvation or hydration numbers in aqueous electrolyte solutions at infinity dilution. The corresponding values are given in Table 1.

Also, Luck (*21*) has measured the solvation number by using optical methods, obtaining $m = 2.83$ at an initial lithium bromide concentration of $x°_{LiBr} = 0.2374$. This coincides very well with the corresponding value $m = 2.81$ resulting from eq 13; see ref 19. Considering the values given by eq 13 and those in Table 1, one can find that the solvation numbers m measured by X-ray studies and those determined by Monte Carlo studies or with a corrected Stoke's radii are somewhat higher than the values of m in eq 13. Marcus defined some important concepts about ion solvation in the liquid phase. The first solvation shell is the set of solvent molecules which are immediate neighbors of the ions. They may interact strongly with the ion. Those molecules which actually do so form the inner coordination sphere (primary solvation). The second solvation shell is the set of solvent molecules which are next-nearest neighbors of the ion. Due to their interaction with the ion they generally have some properties different from those of the bulk solvent molecules. We are not going into details here but refer to the literature (*22*). We are trying to describe the strong interactions between the ions and the solvent molecules with a quasi-chemical reaction forming kind of primary solvation. The second solvation shell and part of the first shell can be described by a local composition model such as, for example, the nonrandom two-liquid model (NRTL) of Renon and Prausnitz (*23*).

The next problem is to relate the solvation numbers $m^{\pm}$ and $n^{\pm}$ in a mixture of two solvents and one salt to the initial concentrations of the components ammonia, water, and lithium bromide. Fitting analytic and experimental VLE data over wide ranges of temperature and concentration, we found the relations

$$m + n = 4 - 5x^\circ_{\mathrm{LiBr}} \tag{14}$$

$$\frac{n^+}{m^+} = a^+(x^\circ_{\mathrm{NH_3}}/x^\circ_{\mathrm{H_2O}})x^\circ_{\mathrm{LiBr}} \tag{15}$$

$$\frac{n^-}{m^-} = a^-(x^\circ_{\mathrm{NH_3}}/x^\circ_{\mathrm{H_2O}})x^\circ_{\mathrm{LiBr}} \tag{16}$$

$$\frac{n^+ + m^+}{n^- + m^-} = \hat{a} \tag{17}$$

to be useful for this purpose. They include the solvation reactions in the corresponding binary systems LiBr + H_2O and LiBr + NH_3 already used in the literature (*9*, *19*) as special cases. The parameters a^+ and a^- are assumed to depend on temperature:

$$a^+ = a_o^+ \exp(-a_e^+/RT) \tag{18}$$

$$a^- = a_o^- \exp(-a_e^-/RT) \tag{19}$$

The parameter $\hat{a}$ is assumed to be constant. Numerical values of all parameters a_o^+, a_e^+, a_o^-, a_e^-, and $\hat{a}$ have been determined by fitting experimental VLE data of the system. They are given in Table 2. For more details about the mixed-solvent solvation model see ref 9.

The solvation numbers $m^\pm$ and $n^\pm$ obtained by the optimization procedure indicate that the anion Br^- is solvated preferentially by ammonia molecules and the cation Li^- by water molecules. This is confirmed by spectroscopic measurements in liquid mixtures of two solvents and one salt of Covington and Dunn (*24*), Sacco et. al (*25*), and Eaton et al. (*26*).

Association Model. The model also includes an association reaction of ammonia and water molecules, forming a second species of clusters. The quasi-chemical reaction of the association is

$$r\mathrm{NH_3} + q\mathrm{H_2O} \rightleftarrows (\mathrm{NH_3})_r(\mathrm{H_2O})_q \tag{20}$$

Mironov (*27*) reported two solid hydrates of ammonia, $NH_3 \cdot H_2O$ and $2NH_3 \cdot H_2O$. Heidemann and Rizvi (*28*) successfully introduced both hydrates in a cubic equation of state describing vapor–liquid equilibria in the ammonia–water system.

Law of Mass Action. The quasi-chemical reactions 5 and 20 lend to the laws of mass action:

$$K_\mathrm{A} = \frac{(\gamma_\mathrm{A} x_\mathrm{A})}{(\gamma_\mathrm{H_2O} x_\mathrm{H_2O})^q (\gamma_\mathrm{NH_3} x_\mathrm{NH_3})^r} \tag{21}$$

$$K_\mathrm{KA} = \frac{(\gamma_{\mathrm{A}^-} x_{\mathrm{A}^-})(\gamma_{\mathrm{K}^-} x_{\mathrm{K}^-})}{(\gamma_\mathrm{LiBr} x_\mathrm{LiBr})(\gamma_\mathrm{NH_3} x_\mathrm{NH_3})^n (\gamma_\mathrm{H_2O} x_\mathrm{H_2O})^m} \tag{22}$$

Here K_i (i = A, KA) is the equilibrium constant, the temperature dependence of which usually can be described by the van't Hoff relation

$$K_i = K_i^\circ \exp[-\Delta H_i^\circ/RT] \tag{23}$$

Table 3. Optimal Parameters for the Equilibrium Constants in the Systems NH_3 + H_2O, H_2O + LiBr, and NH_3 + LiBr

reaction	eq	$\ln K_i^\circ$	ΔH_i°/(J mol^{-1})
association	20	−3.8196	−13 359.92
solvation (C)	12	−5.7953	−49 651.14
solvation (Z)	24	−0.3143	−5 728.00

where ΔH_i° is the standard enthalpy of formation. The equilibrium constant K_KA of reaction 20 is determined by an optimization procedure fitting experimental VLE data of the system NH_3 + H_2O to the association model described below. To model the equilibrium constant K_KA, we call to mind that the stoichiometric eq 5 indicates as limiting reactions for vanishing ammonia reaction 12 and for vanishing water the solvation reaction for the NH_3 + LiBr system:

$$n\mathrm{NH_3} + \mathrm{LiBr} \rightleftarrows \mathrm{Li^+(NH_3)}_{n^-} + \mathrm{Br^-(NH_3)}_{n^-} \tag{24}$$

To ensure the equilibrium constants K_C and K_Z of reactions 12 and 24 to be included as limiting values in K_KA, we assume for the reference values K_KA°, K_Z°, and K_C° the following relation to hold:

$$\ln K_\mathrm{KA}^\circ = \frac{m}{m+n} \ln K_\mathrm{C}^\circ + \frac{n}{m+n} \ln K_\mathrm{Z}^\circ \tag{25}$$

Likewise for the corresponding reaction enthalpies ΔH_i° we assume

$$\Delta H_\mathrm{KA}^\circ = \frac{m}{m+n} \Delta H_\mathrm{C}^\circ + \frac{n}{m+n} \Delta H_\mathrm{Z}^\circ \tag{26}$$

Since VLE data of the system NH_3 + LiBr are lacking, the parameters K_Z°, $\Delta H_\mathrm{Z}^\circ$ are unknown quantities which actually were determined by fitting VLE data of the ternary system NH_3 + H_2O + LiBr to the model discussed. Numerical values are given in Table 3.

Balance Equations. During formation of the ionic clusters, the mole fractions of water $x^\circ_\mathrm{H_2O}$, ammonia $x^\circ_\mathrm{NH_3}$, and lithium bromide x°_LiBr initially being realized in the liquid phase are changed. Also, we have to take into account that due to the condition of electroneutrality the mole fraction of both types of ionic clusters have to be equal:

$$x_\mathrm{K}^+ = x_\mathrm{A}^- = x_\mathrm{k} \tag{27}$$

Denoting by $x_\mathrm{H_2O}$, x_LiBr, x_NH3, and x_k the mole fractions of the respective components after solvation, from the balance equations of mole numbers the following relations can be derived:

$$x_\mathrm{NH_3} = x^\circ_\mathrm{NH_3} + x_\mathrm{k}((m + n - 1)x^\circ_\mathrm{NH_3} - n) + x_\mathrm{A}((r + q - 1)x^\circ_\mathrm{NH_3} - r) \tag{28}$$

$$x_\mathrm{H_2O} = x^\circ_\mathrm{H_2O} + x_\mathrm{k}((m + n - 1)x^\circ_\mathrm{H_2O} - m) + x_\mathrm{A}((r + q - 1)x^\circ_\mathrm{H_2O} - q) \tag{29}$$

$$x_\mathrm{LiBr} = x^\circ_\mathrm{LiBr} + x_\mathrm{k}((m + n - 1)x^\circ_\mathrm{LiBr} - 1) + x_\mathrm{A}(r + q - 1)x^\circ_\mathrm{LiBr} \tag{30}$$

G^E Model. The activities of the various components in the liquid phase are modeled by NRTL equations. Restricting salt concentrations to be high (>5 mass %) in the liquid phase, a Debye–Hückel expression can be neglected. Taking the consistency conditions of Acree (*29*) into account, the number of parameters to be optimized can be reduced considerably. More details about these conditions are given by Peters (*9*). In Tables 4 and 5 the optimal parameters of our calculations are given for the NRTL equation. It should be noted that the parameters α_{ij} and $g_{ij} - g_{ii}$ (i or j equal to K^+ or A^-) in the NRTL equation depend on the composition of ammonia and water in the solvation shell (primary solvation). Therefore, we have

Table 4. Optimal Parameters α_{ij} for NRTL Activities

i/j	H_2O	LiBr	$C^{\pm}$	NH_3	A	$Z^{\pm}$
H_2O	0	0.651	0.170	0.126	0.006	0.001
LiBr	0.651	0	0	0.819	0.003	0
$C^{\pm}$	0.170	0	0	0.041	0.036	0
NH_3	0.126	0.819	0.041	0	5.626	0
A	0.006	0.003	0.036	5.626	0	1.883
$Z^{\pm}$	0.001	0	0	0	1.883	0

Table 5. Optimal Parameters $g_{ij} - g_{jj}$ (J mol^{-1})

i/j	H_2O	LiBr	$C^{\pm}$	NH_3	A	$Z^{\pm}$
H_2O	0	−13 728	−6 206	−5 029	−17 358	−22 979
LiBr	−6 878	0	0	51 081	−49	0
$C^{\pm}$	644	0	0	4 579	46 450	0
NH_3	30 516	79 785	33 274	0	1 750	−26 826
A	16 295	26 754	73 252	−142	0	37 119
$Z^{\pm}$	−16 128	0	0	−55 521	10 317	0

formulated linear mixing rules in *m* and *n* for these parameters; see ref 9.

Results

Water + Lithium Bromide System. Describing vapor−liquid equilibria in the system water + lithium bromide, the solvation model includes seven parameters fitted to 388 experimental data points taken from the literature in the ranges 0.00015−0.316 MPa, 273−463 K, and 5−76 wt % LiBr. The system's pressure resulting from a $(T, x) \rightarrow p$ calculation procedure can be represented with a mean relative deviation of less than 1.4%. More information about the underlying data base and the application of the solvation model in the system H_2O + LiBr is given in refs 9 and 19. Table 6 shows some results for measured vapor pressure data taken from the literature (*30−32*). As a result of this paper we present a new phase diagram (p, x°_{LiBr}) of the LiBr + H_2O system. In Figure 2 vapor pressure data of Renz (*30*) and Löwer (*31*) are plotted. The lines represent isotherms resulting from the solvation model proposed, with fitting parameters given in Tables 4 and 5.

Ammonia + Water System. In a way similar to that of the solvation number *m* of the system H_2O + LiBr, the associating numbers *r* and *q* of the system NH_3 + H_2O, eq 20, were obtained to be $r = 1$ and $q = 1$, indicating that water and ammonia tend to form most often bimolecular clusters! ($NH_3{\cdot}H_2O \cong NH_4OH$). Using the NRTL equation for the activity coefficients, the model includes 10 parameters. These parameters were fitted to 679 experimental data points of VLE in NH_3 + H_2O in the ranges 0.0025−18.57 MPa and 293−503 K taken from the literature (*33−40*). The system's pressure and the concentration of ammonia in the vapor phase resulting from a $(T, x) \rightarrow (p, y)$ calculation procedure can be represented with mean relative deviations of less than 2.78% and 1.99%, respectively. As a result of these calculations we present a phase diagram of the NH_3 + H_2O system. In Figure 3 the vapor pressure data of Gillespie et. al. (*39*), Clifford and Hunter (*37*), Perman (*33*, *34*), and others are plotted against the mole fractions of ammonia in the liquid and the vapor phases. The lines represent isotherms resulting from the associating model proposed. Table 7 shows a comparison between measured vapor−liquid equilibrium data taken from the literature and data calculated with the association model presented here. More details about this model and the underlying data base, including approximately 1500 data points, are given in the literature (*9*, *41*). Here also information on the molecular structure of liquid mixtures of ammonia and water resulting from the model proposed are given.

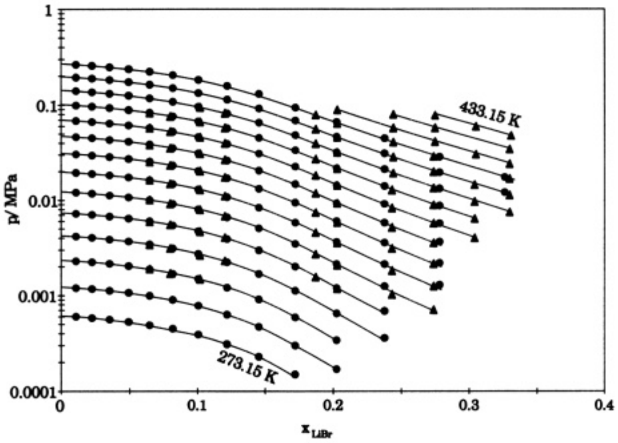

Figure 2. Vapor pressures of H_2O + LiBr: (▲) data of Renz (*31*); (●) data of Löwer (*30*); (−) solvation model (273.15 K ≤ *T* ≤ 433.15 K, Δ*T* = 10 K).

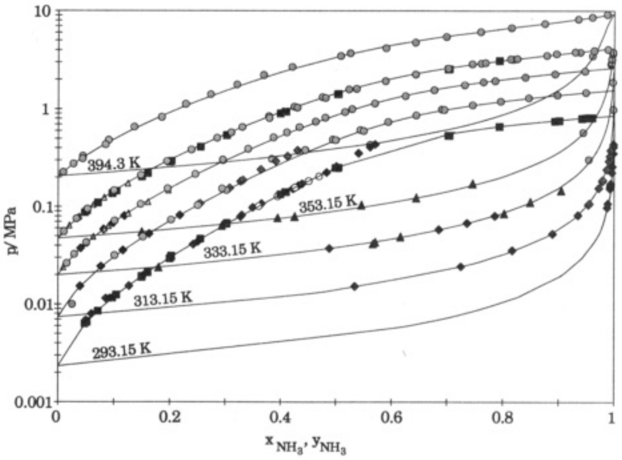

Figure 3. Phase diagram of the system NH_3 + H_2O: (shaded ○) data of Gillespie et al. (*39*); (▲) data of Clifford and Hunter (*37*); (◆) data of Perman (*33*, *34*); (○) data of Foote (*35*); (shaded ◇) data of Patrick and Neuhausen (*36*); (■) data of Smolen et al. (*39*); (−) association model.

Ammonia + Water + Lithium Bromide System. Measured VLE data of this system are presented in Tables 8−11 and Figures 4−8. The data in each table are indicated by the measured temperature and the composition of the liquid phase. In Tables 10 and 11 the measured temperature (|Δ*T*| < 0.2 K) is replaced by an average

Table 6. Sets of Experimental Data of the Vapor Pressure and Statistical Parameters f_m and σ Resulting from a Correlation of These Data to the Solvation Model of Peters and Keller

author	$100f_m$; 100σ	*p*/MPa	*T*/K	$100w_{LiBr}$
Renz	1.16; 1.61	0.00052−0.0948	293.15−448.15	25.10−70.45
Löwer	1.21; 1.92	0.00015−0.264	273.15−403.15	5.00−70.00
Feuerecker	1.49; 1.76	0.0045−0.18	318.25−463.09	40.35−75.97

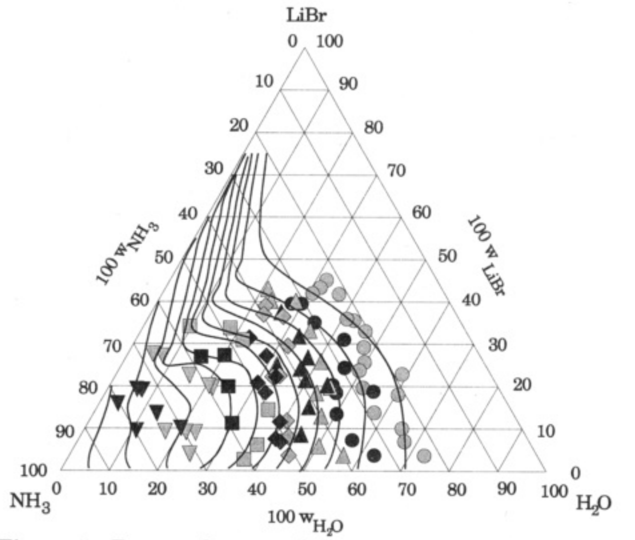

Figure 4. Ternary diagram of the system ammonia + water + lithium bromide presenting isobars of the liquid state at 303.15 K: (shaded ○) 0.1 MPa; (●) 0.2 MPa; (shaded △) 0.3 MPa; (▲) 0.4 MPa; (shaded ◇) 0.5 MPa; (◆) 0.6 MPa; (shaded □) 0.7 MPa; (■) 0.8 MPa; (shaded ▽) 0.9 MPa; (▼) 1.0 MPa.

Table 7. Sets of Selected Experimental Data of the Vapor Pressure, Composition, and Statistical Parameters f_m and σ Resulting from a Correlation of These Data to the Association Model of Peters and Keller

author	$100f_{mp}$; $100\sigma_{mp}$	$100f_{my}$; $100\sigma_{my}$
Gillespie et al. (T < 503 K)	2.26; 3.29	0.94; 1.79
Müller	3.13; 3.68	3.16; 3.71
Clifford and Hunter	1.88; 2.64	2.74; 3.56
Perman	1.57; 2.35	0.49; 0.65
Smolen	2.34; 2.95	

Table 8. Ammonia + Water + Lithium Bromide Equilibrium Data, Average Temperature 374.72 K: Comparison between Calculated and Experimental VLE Data

T/K	x_{NH_3}	x_{LiBr}	p_{meas}/MPa	p_{calc}/MPa	y_{NH_3}-(meas)	y_{NH_3}-(calc)
373.2	0.0002	0.0138	0.061	0.099		0.0034
374.9	0.1142	0.0101	0.282	0.354	0.2424	0.7346
374.8	0.1653	0.0093	0.476	0.506	0.6509	0.8254
374.7	0.2790	0.0089	0.674	0.963	0.7284	0.9205
374.7	0.0002	0.0138	0.884	1.149	0.8001	0.9365
374.7	0.1142	0.0101	1.106	1.176	0.8608	0.9383
374.7	0.3531	0.0077	1.253	1.358	0.9263	0.9488
374.6	0.3866	0.0071	1.459	1.567	0.9688	0.9578
374.7	0.0007	0.0327	0.062	0.101	0.0029	0.0249
374.7	0.0663	0.0316	0.274	0.251	0.3419	0.6363
374.7	0.1313	0.0251	0.490	0.452	0.6644	0.8098
374.7	0.1824	0.0295	0.888	0.688	0.9479	0.8865
374.9	0.3197	0.0244	1.450	1.424		0.9537
375.0	0.0136	0.0501	0.111	0.122	0.7637	0.2411
375.0	0.0790	0.0477	0.260	0.298	0.9167	0.7146
375.1	0.1011	0.0468	0.347	0.382	0.9088	0.7836
374.9	0.1350	0.0403	0.444	0.515	0.9496	0.8445
374.9	0.1745	0.0384	0.583	0.701	0.9462	0.8916
375.1	0.2343	0.0391	0.747	1.057	0.9569	0.9343
375.1	0.2376	0.0374	0.940	1.063	0.9586	0.9345
375.2	0.2617	0.0384	1.117	1.234	0.9647	0.9457
374.7	0.2788	0.0345	1.290	1.290	0.9748	0.9493
374.9	0.3190	0.0302	1.469	1.518		0.9581
374.5	0.0249	0.0699	0.115	0.112	0.4721	0.2666
374.7	0.0611	0.0650	0.198	0.212	0.6647	0.6240
374.5	0.0739	0.0627	0.407	0.258	0.8386	0.6966
374.5	0.1012	0.0645	0.603	0.361	0.8782	0.7956
374.5	0.1992	0.0594	0.721	0.894	0.9202	0.9282
374.5	0.1488	0.0613	0.842	0.599	0.9298	0.8849
374.5	0.1921	0.0524	1.014	0.845	0.9307	0.9202

temperature at the top of these tables. In each table one can find the measured and the calculated vapor pressures.

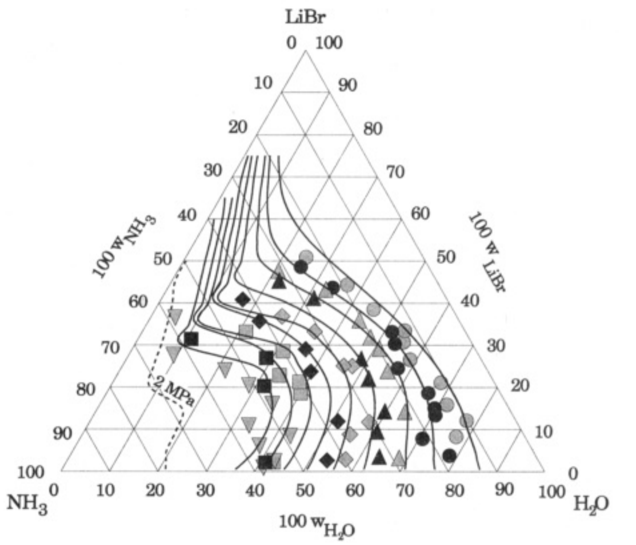

Figure 5. Ternary diagram of the system ammonia + water + lithium bromide presenting isobars of the liquid state at 333.15 K: (shaded ○) 0.1 MPa; (●) 0.2 MPa; (shaded △) 0.3 MPa; (▲) 0.5 MPa; (shaded ◇) 0.7 MPa; (◆) 0.9 MPa; (shaded □) 1.1 MPa; (■) 1.3 MPa; (shaded ▽) 1.5 MPa. Extrapolated pressure: 2 MPa.

Table 9. Ammonia + Water + Lithium Bromide Equilibrium Data, Average Temperature 427.44 K: Comparison between Calculated and Experimental VLE Data

T/K	x_{NH_3}	x_{LiBr}	p_{meas}/MPa	p_{calc}/MPa	y_{NH_3}-(meas)	y_{NH_3}-(calc)
420.5	0.0050	0.0746	0.262	0.401	0.0076	0.1445
426.3	0.0134	0.0863	0.410	0.476	0.2700	0.2188
426.6	0.0382	0.0938	0.520	0.600		0.4251
426.7	0.0792	0.1093	0.715	0.772	0.6431	0.6304
426.8	0.1211	0.1013	0.951	1.496	0.7244	0.8073
426.7	0.1355	0.0985	1.163	1.755	0.8398	0.8349
426.7	0.1475	0.0927	1.360	2.059	0.8369	0.8534
426.9	0.1690	0.0877	1.548	2.490	0.8682	0.8750
430.4	0.0503	0.1709	0.329	0.241	0.7456	
430.5	0.0989	0.1614	0.472	0.329	0.7530	0.3978
430.4	0.1272	0.1610	0.717	0.473	0.8889	0.6236
430.3	0.1652	0.1515	0.878	0.809	0.9422	0.7851
430.3	0.1645	0.1454	1.071	0.904	0.7334	0.7958
430.2	0.1748	0.1440	1.249	0.999	0.8305	0.8171
430.1	0.1809	0.1367	1.480	1.204	0.9159	0.8384
426.7	0.1010	0.1696	0.381	0.269		0.3746
427.3	0.1461	0.1694	0.493	0.467	0.6985	0.6903
427.3	0.1589	0.1779	0.602	0.471	0.5754	0.7232
427.2	0.1519	0.1702	0.805	0.488	0.7837	0.7110
427.1	0.1162	0.0945	0.942	1.588	0.7934	0.8041
427.1	0.1688	0.1546	1.145	0.719	0.8551	0.7868
427.3	0.1851	0.1596	1.323	0.749	0.8957	0.8105
422.8	0.0002	0.1997	0.095	0.211	0.0021	
427.1	0.0041	0.1818	0.216	0.253	0.5739	
427.0	0.0247	0.1291	0.391	0.297	0.7585	
428.9	0.1166	0.1561	0.601	0.429	0.7954	0.5700
427.2	0.1637	0.1435	0.749	0.854	0.8705	0.7977
427.1	0.1753	0.1402	0.922	0.994	0.8897	0.8248
427.1	0.1940	0.1353	1.083	1.237	0.9107	0.8566
427.1	0.2044	0.1338	1.230	1.350	0.9164	0.8688
427.2	0.2500	0.1354	1.372	1.605	0.9317	0.8993
427.1	0.2434	0.1234	1.585	1.989	0.9222	0.9042

Due to corrosion problems in the gas circuit, the vapor composition only could be measured at 373.15 and 423.15 K. The calculated vapor composition is reported for all data points, indicating that at lower temperatures ($T \leq 333.15$ K) the vapor phase contains only small amounts of water. Figure 4 shows the phase diagram of the ammonia + water + lithium bromide system at 303.15 K. The vapor pressure data are correlated by the mixed-solvent solvation model in the range 0.1−1.1 MPa and at salt concentrations of up to 75 mass % LiBr.

Table 10. Ammonia + Water + Lithium Bromide Equilibrium Data, Temperature 333.15 K: Comparison between Calculated and Experimental VLE Data

x_{NH_3}	x_{LiBr}	p_{meas}/MPa	p_{calc}/MPa	y_{NH_3}(meas)	y_{NH_3}(calc)	x_{NH_3}	x_{LiBr}	p_{meas}/MPa	p_{calc}/MPa	y_{NH_3}(meas)	y_{NH_3}(calc)
0.0722	0.0075	0.100	0.060	0.7427	0.6762	0.1933	0.0835	0.102	0.158		0.9390
0.1929	0.0093	0.200	0.160	0.9409	0.9060	0.2199	0.0819	0.199	0.207		0.9556
0.3049	0.0093	0.300	0.337	0.9628	0.9647	0.2674	0.0777	0.301	0.314		0.9729
0.3472	0.0106	0.500	0.442	0.9861	0.9761	0.3254	0.0695	0.500	0.488		0.9840
0.4212	0.0098	0.706	0.667	0.9964	0.9871	0.3551	0.0635	0.703	0.600		0.9875
0.4615	0.0094	0.900	0.817		0.9907	0.4664	0.0591	0.924	1.019		0.9943
0.5746	0.0101	1.106	1.325		0.9961	0.4982	0.0515	1.101	1.182		0.9954
0.5913	0.0099	1.300	1.398		0.9964	0.4855	0.0431	1.506	1.146		0.9950
0.6983	0.0119	1.312	1.835		0.9981	0.1772	0.0936	0.107	0.109		0.9155
0.5954	0.0042	1.499	1.324		0.9960	0.2156	0.0921	0.200	0.167		0.9489
0.1601	0.0182	0.105	0.134	0.8615	0.8858	0.2829	0.0871	0.301	0.306		0.9748
0.2391	0.0170	0.201	0.239	0.9426	0.9452	0.3772	0.0750	0.500	0.610		0.9889
0.3219	0.0109	0.700	0.381		0.9705	0.5149	0.0614	0.906	1.193		0.9957
0.5852	0.0105	1.106	1.379		0.9963	0.5462	0.0561	1.132	1.349		0.9964
0.6764	0.0110	1.303	1.761		0.9979	0.5852	0.0485	1.301	1.533		0.9971
0.1185	0.0313	0.100	0.097		0.8410	0.6224	0.0488	1.502	1.654		0.9975
0.1877	0.0376	0.200	0.191		0.9324	0.2457	0.1134	0.103	0.139		0.9537
0.2131	0.0277	0.300	0.219		0.9410	0.2979	0.1027	0.334	0.254		0.9745
0.3366	0.0312	0.615	0.518		0.9824	0.4308	0.0953	0.500	0.591		0.9914
0.4218	0.0456	0.935	0.875		0.9924	0.4376	0.0913	0.704	0.649		0.9920
0.4306	0.0289	1.164	0.855		0.9918	0.4704	0.0762	0.899	0.902		0.9941
0.6016	0.0314	1.500	1.610		0.9973	0.5323	0.0743	1.119	1.134		0.9960
0.1494	0.0373	0.100	0.135		0.8955	0.5767	0.0690	1.305	1.341		0.9969
0.1827	0.0351	0.200	0.181		0.9267	0.6814	0.0591	1.513	1.712		0.9981
0.2572	0.0328	0.300	0.314		0.9644	0.3035	0.1394	0.103	0.125		0.9684
0.3051	0.0329	0.503	0.432		0.9773	0.3541	0.1356	0.200	0.180		0.9802
0.3500	0.0262	0.700	0.536		0.9830	0.3765	0.1338	0.300	0.211		0.9837
0.3843	0.0254	0.905	0.648		0.9873	0.4199	0.1242	0.504	0.315		0.9891
0.4183	0.0217	1.103	0.752		0.9898	0.5243	0.1049	0.703	0.706		0.9954
0.5337	0.0181	1.499	1.233		0.9955	0.5896	0.0999	0.900	0.916		0.9971
0.1393	0.0523	0.100	0.121		0.8905	0.6289	0.0901	1.100	1.157		0.9977
0.1827	0.0450	0.203	0.187		0.9333	0.7771	0.0831	1.299	1.305		1.0000
0.3017	0.0475	0.311	0.455		0.9800	0.8164	0.0700	1.520	1.642		1.0000
0.3689	0.0371	0.501	0.652		0.9877	0.4192	0.1731	0.108	0.139		0.9901
0.5004	0.0370	0.702	1.206		0.9954	0.4445	0.1600	0.205	0.187		0.9919
0.4884	0.0355	0.943	1.146		0.9950	0.5203	0.1547	0.301	0.269		0.9966
0.5754	0.0278	1.191	1.496		0.9969	0.5216	0.1426	0.541	0.323		0.9961
0.6086	0.0286	1.311	1.625		0.9974	0.6383	0.1208	0.914	0.590		0.9986
0.6233	0.0239	1.501	1.660		0.9975	0.6838	0.1170	1.300	0.621		0.9997
0.1947	0.0692	0.102	0.192		0.9452	0.8292	0.1016	1.498	1.885		1.0000
0.2366	0.0623	0.217	0.286		0.9652	0.5946	0.0057	1.300	1.349		0.9962
0.2652	0.0604	0.310	0.354		0.9735	0.5953	0.0017	1.499	1.281		0.9957
0.3208	0.0547	0.506	0.511		0.9836	0.5713	0.0049	1.500	1.235		0.9954
0.3766	0.0546	0.704	0.694		0.9895	0.1601	0.0182	0.105	0.134		0.8858
0.4957	0.0468	0.917	1.181		0.9953	0.3220	0.0109	0.700	0.381		0.9705
0.4990	0.0439	1.101	1.202		0.9954	0.6251	0.0090	1.504	1.533		0.9971
0.5687	0.0367	1.500	1.494		0.9968						

Table 11. Ammonia + Water + Lithium Bromide Equilibrium Data, Temperature 303.15 K: Comparison between Calculated and Experimental VLE Data

x_{NH_3}	x_{LiBr}	p_{meas}/MPa	p_{calc}/MPa	y_{NH_3}(calc)	x_{NH_3}	x_{LiBr}	p_{meas}/MPa	p_{calc}/MPa	y_{NH_3}(calc)
0.2509	0.0076	0.103	0.073	0.9624	0.4903	0.1163	0.217	0.184	0.9973
0.3588	0.0077	0.197	0.168	0.9881	0.6183	0.0840	0.602	0.529	0.9992
0.4237	0.0077	0.306	0.255	0.9942	0.6836	0.0695	0.824	0.708	0.9995
0.5412	0.0075	0.504	0.487	0.9982	0.8659	0.0200	0.991	0.985	0.9998
0.6352	0.0054	0.710	0.677	0.9992	0.3665	0.1427	0.095	0.055	0.9899
0.2835	0.0150	0.105	0.100	0.9768	0.3382	0.1273	0.096	0.062	0.9873
0.3984	0.0156	0.202	0.237	0.9937	0.5199	0.1034	0.501	0.277	0.9981
0.4734	0.0125	0.304	0.366	0.9970	0.6358	0.0819	0.709	0.568	0.9993
0.5622	0.0115	0.556	0.554	0.9987	0.7666	0.0545	0.920	0.854	0.9997
0.2800	0.0222	0.099	0.105	0.9786	0.8383	0.0356	1.038	0.954	0.9998
0.3746	0.0216	0.232	0.214	0.9928	0.3926	0.1341	0.099	0.075	0.9924
0.5096	0.0186	0.413	0.469	0.9982	0.5513	0.1190	0.309	0.222	0.9986
0.5382	0.0172	0.496	0.530	0.9986	0.5687	0.1135	0.494	0.266	0.9988
0.5667	0.0161	0.594	0.591	0.9989	0.6711	0.0921	0.707	0.516	0.9995
0.6065	0.0128	0.702	0.663	0.9991	0.8660	0.0698	0.893	0.949	1.0000
0.7471	0.0080	0.923	0.867	0.9996	0.8392	0.0682	0.892	0.851	1.0000
0.7875	0.0050	1.002	0.904	0.9997	0.8863	0.0448	0.998	0.975	1.0000
0.3324	0.0315	0.102	0.171	0.9902	0.8710	0.0444	0.999	0.936	0.9998
0.4216	0.0305	0.210	0.313	0.9963	0.4852	0.0065	0.504	0.363	0.9969
0.4577	0.0291	0.300	0.384	0.9974	0.5568	0.0145	0.594	0.562	0.9987
0.5193	0.0278	0.441	0.517	0.9985	0.5871	0.0222	0.508	0.655	0.9991
0.5381	0.0261	0.508	0.556	0.9987	0.6335	0.0203	0.654	0.742	0.9993
0.6335	0.0203	0.654	0.742	0.9993	0.3197	0.0449	0.202	0.164	0.9903
0.4121	0.0438	0.202	0.305	0.9963	0.7317	0.0090	1.001	0.857	0.9996
0.4832	0.0346	0.397	0.446	0.9980	0.4222	0.0476	0.297	0.324	0.9967

Table 11 (Continued)

x_{NH_3}	x_{LiBr}	p_{meas}/MPa	p_{calc}/MPa	y_{NH_3}(calc)
0.5541	0.0255	0.606	0.591	0.9989
0.6506	0.0197	0.857	0.770	0.9994
0.6750	0.0098	1.001	0.783	0.9994
0.3431	0.0473	0.104	0.196	0.9926
0.4168	0.0490	0.195	0.312	0.9965
0.5265	0.0408	0.462	0.547	0.9986
0.3402	0.0594	0.100	0.187	0.9925
0.4594	0.0435	0.306	0.398	0.9976
0.5207	0.0379	0.549	0.528	0.9986
0.5788	0.0326	0.692	0.652	0.9991
0.6608	0.0246	0.798	0.790	0.9994
0.7597	0.0195	0.924	0.887	0.9996
0.3762	0.0614	0.200	0.233	0.9947
0.4817	0.0522	0.397	0.431	0.9980
0.5834	0.0434	0.612	0.653	0.9991
0.7399	0.0193	0.912	0.870	0.9996
0.8365	0.0136	1.038	0.952	0.9997
0.3202	0.0658	0.099	0.156	0.9907
0.4909	0.0603	0.410	0.429	0.9981
0.6000	0.0499	0.598	0.673	0.9992
0.3107	0.0775	0.104	0.130	0.9891
0.4336	0.0658	0.302	0.314	0.9968
0.5460	0.0551	0.498	0.555	0.9988
0.2918	0.0914	0.103	0.093	0.9851
0.3585	0.0838	0.199	0.166	0.9928
0.4666	0.0688	0.406	0.360	0.9975
0.5549	0.0541	0.591	0.574	0.9989
0.6721	0.0473	0.813	0.794	0.9995
0.7721	0.0218	0.983	0.901	0.9997
0.3354	0.1024	0.101	0.103	0.9893
0.4322	0.0984	0.200	0.200	0.9958
0.4485	0.0911	0.301	0.247	0.9966
0.4815	0.0859	0.407	0.314	0.9976
0.5163	0.0777	0.498	0.408	0.9983
0.5755	0.0696	0.592	0.550	0.9990
0.6442	0.0606	0.761	0.707	0.9994
0.7178	0.0475	0.906	0.847	0.9996
0.8301	0.0299	0.995	0.956	0.9998
0.8874	0.0205	1.084	1.008	0.9998
0.4216	0.1275	0.101	0.102	0.9944
0.5265	0.0408	0.462	0.547	0.9986
0.7425	0.0273	0.700	0.883	0.9996
0.7842	0.0277	0.804	0.917	0.9997
0.8047	0.0197	0.900	0.929	0.9997
0.6872	0.0307	0.692	0.829	0.9995
0.4299	0.0490	0.397	0.336	0.9969
0.5379	0.0291	0.716	0.561	0.9987
0.5483	0.0621	0.410	0.534	0.9988
0.5632	0.0542	0.494	0.590	0.9989
0.6275	0.0522	0.598	0.715	0.9993
0.4910	0.0629	0.302	0.423	0.9980
0.7090	0.0464	0.906	0.841	0.9996
0.9704	0.0231	1.084	1.131	1.0000
0.6756	0.0789	0.602	0.632	0.9995
0.7045	0.0631	0.716	0.766	0.9996
0.9219	0.0355	0.991	1.058	1.0000
0.4761	0.1190	0.300	0.163	0.9969
0.5650	0.0068	0.398	0.534	0.9986
0.7643	0.0097	0.681	0.878	0.9996
0.8096	0.0081	0.748	0.922	0.9997
0.8610	0.0051	0.872	0.978	0.9998
0.7786	0.0175	0.762	0.903	0.9997
0.2618	0.0429	0.101	0.102	0.9804
0.6324	0.0351	0.498	0.750	0.9993
0.9469	0.0164	1.005	1.093	1.0000
0.2327	0.0573	0.098	0.080	0.9746
0.4988	0.0676	0.198	0.421	0.9981
0.5500	0.0629	0.296	0.537	0.9988
0.5725	0.1015	0.293	0.350	0.9988
0.6356	0.0982	0.391	0.437	0.9994
0.6432	0.0803	0.501	0.588	0.9994
0.3156	0.1009	0.101	0.093	0.9872
0.4607	0.1165	0.203	0.159	0.9964
0.5564	0.1312	0.299	0.169	0.9988
0.5242	0.1076	0.398	0.259	0.9981
0.5762	0.1051	0.504	0.321	0.9989
0.6540	0.1128	0.584	0.318	0.9996
0.7821	0.0930	0.715	0.655	1.0000
0.7435	0.0683	0.821	0.758	0.9997

The shape of the correlated isobars fit the data fairly well within the ranges of pressure and concentration investigated. For high concentrations of salt and ammonia, i.e., the water content in the liquid phase is less than 10 mass %, the isobars show a strong bend in the triangular diagram. This behavior can be explained by the appearance of a solid phase, not only indicated by the model but also observed in our experiments (*11*). The model could be extrapolated to correlate VLE data at higher temperatures (T > 303.15 K) also. As can be seen from the triangular phase diagrams the shape of the isobars is nearly congruent and depends on the initial composition of the liquid phase. At 423.15 K the extrapolations of the mixed-solvent solvation model show the appearance of a miscibility gap in the middle of the triangular phase diagram. At constant lithium bromide concentration a fixed vapor pressure p can be obtained by three different weight fractions of ammonia in the liquid phase. Two of them could be equilibrium states on the phase envelope of the miscibility gap; the third composition must be instable. These limiting compositions are not identical with connodes of a state of liquid–liquid equilibrium. The conditions of liquid–liquid equilibrium has not been proven yet. This task is being left for future investigations.

In the lower part of Figure 7 the corresponding vapor phase and its pressure and composition are shown. As an example, a special vapor–liquid equilibrium state at 2 MPa and 40 mass % LiBr in water is indicated by a dashed line. The phase diagrams show that the data correlation is in fairly good agreement with the measured data points. The mean deviation between the correlated and the experimental data seems to be somewhat smaller than the dispersion of the data themselves. Correlating the experimental data points, the mean relative deviation in pressure amounts to 14%. The comparison between interpolations of the experimental data and the data from the mixed-solvent solvation model leads to relative deviations of 5.3% (Δp = 53 kPa). At 373 K and high salt concentrations (>30 mass

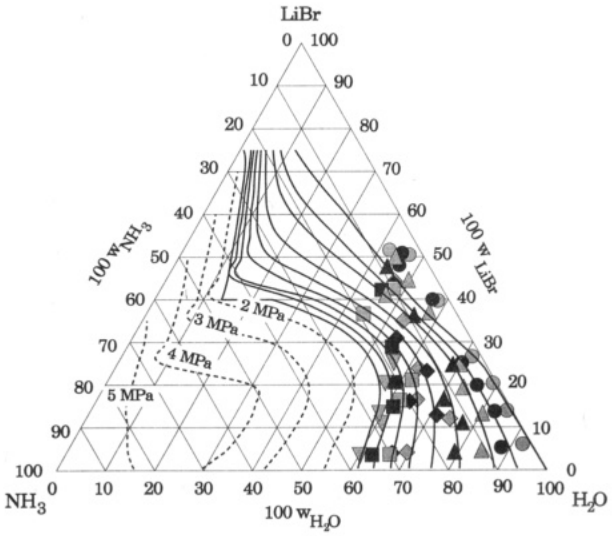

Figure 6. Ternary diagram of the system ammonia + water + lithium bromide presenting isobars of the liquid state at 373.15 K: (shaded ○) 0.1 MPa; (●) 0.2 MPa; (shaded △) 0.3 MPa; (▲) 0.5 MPa; (shaded ◇) 0.7 MPa; (◆) 0.9 MPa; (shaded □) 1.1 MPa; (■) 1.3 MPa; (shaded ▽) 1.5 MPa. Extrapolated pressures: 2–5 MPa.

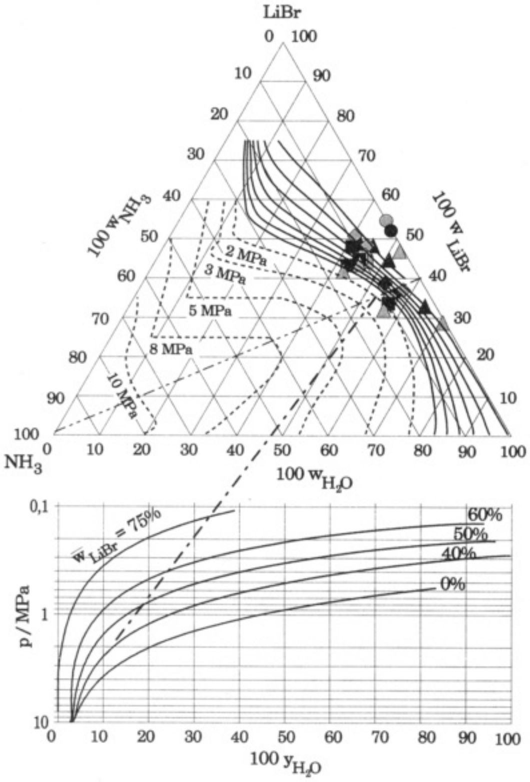

Figure 7. Ternary diagram of the system ammonia + water + lithium bromide presenting isobars of the liquid state at 423.15 K: (shaded ○) 0.1 MPa; (●) 0.2 MPa; (shaded △) 0.3 MPa; (▲) 0.5 MPa; (shaded ◇) 0.7 MPa; (◆) 0.9 MPa; (shaded □) 1.1 MPa; (■) 1.3 MPa; (shaded ▽) 1.5 MPa. Extrapolated pressures: 2, 3, 5, 8, 10 MPa. The lower part of the diagram shows the corresponding vapor states (p, y_{H_2O}) indicated by the initial concentration of lithium bromide in the liquid phase of LiBr + H_2O.

% LiBr in water) the measured data points in Figure 7 indicate systematic deviations from the correlated VLE data, obviously due to experimental errors. These data are not included in Table 8. More information about the data scattering is given by Zimmermann (*7*) and Peters (*9*).

Comparison with Other Results. Figure 8 presents the current results of Radermacher (*5*) at a constant lithium bromide concentration of 60 mass % referring to the system H_2O + LiBr. The lines in Figure 8 represent the data correlation of the corresponding experimental data with the mixed-solvent solvation model. Correlating the experimental data points, the mean relative deviation in pressure amounts to 2.44% (Δp = 43 kPa) and the mean relative deviation amounts to 3.03% (Δy = 0.0245) for the mole fraction of ammonia in the vapor phase. The left hand side of Figure 8 illustrates the (p, T) behavior for several solutions with known mole fractions (referring to the system $NH_3 + H_2O$) of ammonia in the liquid phase. The right hand side of this figure shows the mole fraction of ammonia in the vapor phase above these solutions. As can be seen the correlations are in good agreement with the experimental data points. Only the deviations between the measured and calculated vapor compositions above solutions with 43.6 and 38.3 mass % ammonia are slightly higher.

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Glossary

a	parameter of the EOS, eq 2
k^-	solvation number for the anion Br^-
a^+	parameter in eq 15
a^-	parameter in eq 16
a_o^+	parameter in eq 18
a_e^+	parameter in eq 18
a_o^-	parameter in eq 19
a_e^-	parameter in eq 19
$\hat{a}$	parameter in eq 17
b	parameter of the EOS, eq 2
f	relative deviation
g_{ij}	molecular energy between molecules of species i and j
K_i	equilibrium constant
$\mathrm{K}_{i\infty}$	equilibrium constant for $T \rightarrow \infty$
k^+	solvation number for the cation Li^+
m	solvation number (water)
n	solvation number (ammonia)
p	pressure
r	association number (ammonia)
p_{oi}	vapor pressure of pure species i
q	association number (water)

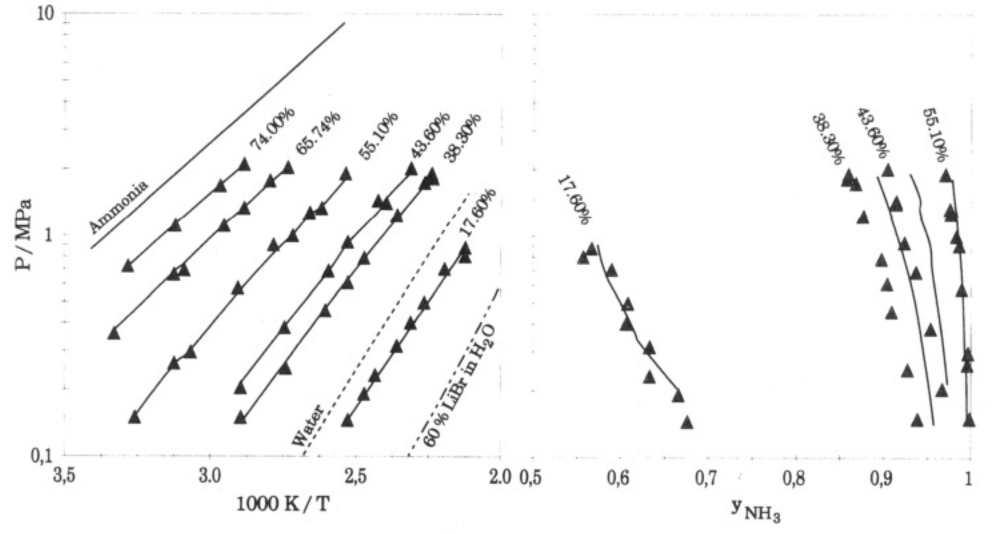

Figure 8. Comparison between the calculated VLE data of this work with the corresponding measured values of Radermacher (*5*) for a solution with a salt concentration of 60 mass % LiBr in water.

R	gas constant
T	temperature
x_i	mole fraction of species i in the liquid phase
y_i	mole fraction of species i in the gas phase
w_i	weight fraction of species i in the liquid phase
v	molar volume
v_{oi}	molar volume of pure species i
Z	compressibility factor
α_{ij}	NRTL's interaction parameter
ΔH°	heat of activation
φ_i	fugacity coefficient of species i
φ_{oi}	fugacity coefficient of pure species i
γ_i	activity coefficient of species i
σ	standard deviation

Subscripts

1	water
2	lithium bromide
3	ionic complex (Li^+)
4	ammonia
5	associate (NH_4OH)
6	ionic complex (Br^-)
c	critical state
A	association
A^-	anion
C	solvation (water)
H_2O	water
K^+	cation
k	complex (both anion and cation)
KA	mixed-solvent solvation
LiBr	lithium bromide
m	average value
mp	average value (pressure)
my	average value (vapor composition)
NH_3	ammonia
Z	solvation (ammonia)

Superscripts

c	critical state
°	state prior to solvation
s	boiling state
+	positive charge
−	negative charge
*	$T = 373$ K

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