Thermodynamic Properties of the NaBr + H_2O System

Donald G. Archer

Electrolyte Data Center, National Institute of Standards and Technology, Gaithersburg, MD 20899

Received May 3, 1990; revised manuscript received September 14, 1990

Equations that described the thermodynamic properties of the NaBr + H_2O system were obtained from a fit to experimental results for this system. The experimental results included in the fit spanned the range of temperature of approximately 260 to 623 K and the range of pressure from the vapor pressure of the solution to 150 MPa. New equations and/or values for the following properties are given in the present work: 1) the change in chemical potential with respect to temperature and pressure for NaBr(cr), valid from 200 to 900 K, 2) $\Delta_f G^\circ_m$ and $\Delta_f H^\circ_m$ for formation from the elements for NaBr(cr) for 298.15 K and 0.1 MPa, 3) $\Delta_f G^\circ_m$ and $\Delta_f H^\circ_m$ from the elements, as well as S°_m and $C^\circ_{p,m}$, all for 298.15 K, 0.1 MPa for $NaBr{\cdot}2H_2O(cr)$, 4) the change in chemical potential for both NaBr and H_2O in NaBr(aq) as a function of temperature, pressure, and molality, valid from 260 to 600 K and from the vapor pressure of the solution to 150 MPa.

Key words: activity coefficient, apparent molar properties, aqueous, compressibility, dehydration, density, enthalpy, equation of state, expansivity, formation properties, Gibbs energy, heat capacity, osmotic coefficient, partial molar properties, sodium bromide, sodium bromide dihydrate, solubility, thermodynamics, vapor pressure.

Contents

1. Introduction 511
2. Thermodynamic Properties of NaBr(cr) 511
3. Thermodynamic Properties of $NaBr{\cdot}2H_2O(cr)$. 512
4. Thermodynamic Properties of NaBr(aq) 513
   4.1. Description of Equations 513
   4.2. Agreement with the Experimental Results for NaBr(aq) 517
      4.2.1. Volumetric Properties 518
      4.2.2. Activity and Thermal Properties ... 521
      4.2.3. Solubilities of $NaBr{\cdot}2H_2O(cr)$ and NaBr(cr) 526
5. $NaBr{\cdot}2H_2O(cr) = NaBr(cr) + 2H_2O(g)$ 532
6. Estimation of Uncertainty and Calculated Values 533
7. Acknowledgment 534
8. References 534

List of Tables

1. Least-Squares Estimated Parameters for Eq. (1). 512
2. Least-Squares Estimated Parameters for Eqs. (5–39). 517
3. Literature sources for the volumetric properties of NaBr(aq). 518
4. Literature sources for the activity and thermal properties of NaBr(aq). 522
5. The 298.15 K, 0.1 MPa Gibbs energy and enthalpy of formation of NaBr(cr) and $NaBr{\cdot}2H_2O(cr)$ 532
6. The enthalpy of solution of NaBr(cr) and $NaBr{\cdot}2H_2O(cr)$ 532

A-1. The calculated standard-state molar Gibbs energy for NaBr(aq) relative to 298.15 K and 0.1 MPa 536
A-2. The calculated standard-state molar enthalpy for NaBr(aq) relative to 298.15 K and 0.1 MPa 536
A-3. The calculated standard-state molar entropy for NaBr(aq) 537
A-4. The calculated activity coefficient for NaBr(aq) 538
A-5. The calculated osmotic coefficient for NaBr(aq) 541
A-6. The calculated apparent molar volume for NaBr(aq) 545
A-7. The calculated density for NaBr(aq) 549
A-8. Calculated values of $\beta^{(0)}_{MX}$ 552
A-9. Calculated values of $\beta^{(1)}_{MX}$ 553
A-10. Calculated values of $C^{(0)}_{MX}$ 554
A-11. Calculated values of $C^{(1)}_{MX}$ 554

List of Figures

1. Weighted residuals from fitting Eq. (1) to the heat-capacity and enthalpy-change measurements for NaBr(cr) against temperature. 513

2. Residuals, in terms of apparent molar volume, for 298.15 K and 0.1 MPa against the square root of molality.......... 519
3. Comparison of values for the difference in density between solution and water, against pressure, for 298.15 K.......... 520
4. The isentropic compressibility calculated from the fitted equation compared with that estimated from measurements of the speed of sound in NaBr(aq) for 298.15 K, 0.1 MPa ... 521
5. Difference between the experimentally observed change in apparent molar heat capacity for a 17.5 MPa change in pressure and that calculated from an equation fitted to the experimental volumetric results 523
6. Comparison of values of the activity coefficient calculated from the fitted equation and the values of Harned and Owen for 4 mol·kg^{-1} NaBr(aq) against temperature.......... 524
7. Residual plot for the osmotic coefficient for temperatures from the freezing point to 298.15 K and from 0 to 2 mol·kg^{-1}.......... 525
8. Residual plot for the osmotic coefficient for temperatures from the freezing point to 298.15 K and from 0 to the saturation molality 525
9. Comparison of the osmotic coefficients calculated from Jakli and Van Hook's vapor pressure measurements to those calculated from the present equation.......... 526
10. Values of the osmotic coefficient from 423.15 to 573.15 K and values of the osmotic coefficients calculated from the vapor-pressure measurements of Mashovets *et al*.......... 527
11. Comparison of fitted equation with the enthalpy of dilution values of Mayrath and Wood.......... 527
12. Residual plot for the fitted heat-capacity measurements for 278.15 to 350.30 K 528
13. Residual plot for the fitted heat-capacity measurements for 400 to 501 K.......... 528
14. Residual plot for the fitted heat-capacity measurements for 552 to 603 K.......... 529
15. The apparent molar heat capacity for a 1.0031 mol·kg^{-1} solution, experiment compared to fitted equation 530
16. Values of the solubility of NaBr(cr) and NaBr·2H$_2$O(cr) calculated from the equation for the solution properties combined with thermodynamic properties of the solid phases from Wagman *et al*.......... 530
17. Values of the solubility of NaBr(cr) and NaBr·2H$_2$O(cr) calculated from the equation for the solution properties combined with thermodynamic properties of the solid phases from the present work.......... 531
18. The difference of the decomposition pressure for NaBr·2H$_2$O(cr) calculated from the present work and experiment.......... 533

List of Symbols

A_ϕ, A_H, A_C, A_V	Debye-Hückel coefficients for osmotic coefficient, apparent molar enthalpy, apparent molar constant-pressure heat capacity and apparent molar volume.
a_w	Activity of water in a solution.
b	A constant in Pitzer's ion-interaction equation, chosen to be 1.2 kg$^{1/2}$·mol$^{-1/2}$.
C_p°	1.0 kJ·mol^{-1}·K^{-1}.
$C_{p,\phi}$	Apparent molar constant-pressure heat capacity.
$C_{p,\mathrm{m},2}^\circ$	Standard-state constant-pressure molar heat capacity of the solute.
$C_{p,\mathrm{m,cr}}^\circ$	Standard-state constant-pressure molar heat capacity of a crystalline phase.
$c_{p,\mathrm{s}}$	Specific constant-pressure heat capacity of a solution.
$c_{p,\mathrm{w}}$	Specific constant-pressure heat capacity of one kg of water.
$C_p(m_\mathrm{r})$	Constant-pressure heat capacity of a quantity of solution of molality m_r and containing one kg of solvent.
$C_\mathrm{MX}, C_\mathrm{MX}^{(0)}, C_\mathrm{MX}^{(1)}$	Ion-interaction parameters for Pitzer's equation.
G	Gibbs energy (extensive).
G^ex	Excess Gibbs energy of a solution (extensive).
$G_\mathrm{m,1}^\circ, G_\mathrm{m,2}^\circ$	Standard-state molar Gibbs energy of the solvent and the solute, respectively.
$G_\mathrm{m,cr}^\circ$	Standard-state molar Gibbs energy of a crystalline phase.
$G_\mathrm{m,1,g}^\circ$	Standard-state molar Gibbs energy of the solvent gas phase.
$H_\mathrm{m,cr}^\circ$	Standard-state molar enthalpy of a crystalline phase.
I	Ionic strength ($I = 0.5\Sigma m_i z_i^2$).
$K_{\phi,\mathrm{s}}^\circ$	Apparent molar isentropic compressibility.
L°	1.0 kJ·mol^{-1}.
L_ϕ	Relative apparent molar enthalpy.
$L_\mathrm{m,1}$	Partial molar enthalpy of the solvent.
M_1	Molar mass of the solvent, 18.0153 × 10^{-3} kg·mol^{-1}.
m	Molality.
m°	1.0 mol·kg^{-1}.
m_r	Reference molality.
n_i	Moles of the i'th substance.
p	Pressure.
p	1.0 MPa
p_w	Vapor pressure of pure water.

p_r	Reference pressure; as a subscript to a property it denotes that the value of the property is that for the reference pressure.
R	Gas constant, 8.3144×10^{-3} $kJ\cdot mol^{-1}$.
S^{ex}	Excess entropy of a solution (extensive).
$S^\circ_{m,\,cr}$	Standard-state molar entropy of a crystalline phase.
$S^\circ_{1,\,m}$, $S^\circ_{2,\,m}$	Standard-state molar entropy of the solvent and the solute.
T	Temperature.
T°	1.0 K
T_r	A reference temperature; as a subscript to a property it denotes that the value of the property is that for the reference temperature.
u	Speed of sound.
V°	$1.0\ cm^3\cdot mol^{-1}$.
V_ϕ	Apparent molar volume.
$V^\circ_{m,\,2}$	Standard-state molar volume of the solute.
$V^\circ_{m,\,cr}$	Standard-state molar volume of a crystalline phase.
$V(m_r)$	Volume of a quantity of solution of molality m_r and containing 1 kg of solvent.
z_M, z_X	The charges of ions M and X.
α	A constant in Pitzer's equation, chosen to be $2.0\ kg^{1/2}\cdot mol^{-1/2}$.
α_s	Expansivity of a solution.
β	Isothermal compressibility.
β_S	Isentropic compressibility.
$\beta^{(0)}_{MX}$, $\beta^{(1)}_{MX}$	Ion-interaction parameters in Pitzer's ion interaction equation.
$\Delta_f G^\circ_m$	The standard-state molar Gibbs energy change for formation from the elements.
$\Delta_{dec} G^\circ_m$	The standard-state molar Gibbs energy change for decomposition of a material.
$\Delta_{sol} G^\circ_{anhydrous}$	The standard-state molar Gibbs energy change for solution of an anhydrous solute.
$\Delta_{sol} G^\circ_{dihydrate}$	The standard-state molar Gibbs energy change for solution of a dihydrate solute.
$\Delta_f H^\circ_m$	The standard-state molar enthalpy change for formation from the elements.
$\Delta_{fus} T$	The difference in freezing point temperature for a solvent from a solution and the pure solvent.
$\Delta_{dil} V_\phi$	The change in apparent molar volume for a change in molality.
$\gamma_\pm$	Stoichiometric activity coefficient of the solute.
ϕ	Osmotic coefficient.
ρ	Density.
ρ°	$1.0\ g\cdot cm^{-3}$.
ν	$\nu_M + \nu_X$
ν_M, ν_X	The stoichiometric number of M and X ions in the electrolyte $M_{\nu_M} X_{\nu_X}$.
v_w	Volume of one kg of water.

1. Introduction

Three equations were used to represent experimental results for the NaBr + H_2O system. These were: 1) the equation of state for water given by Hill[1]; 2) an equation for the change in chemical potential of NaBr(cr) as a function of temperature and pressure; and 3) an equation for the changes in chemical potentials for the aqueous solution. The equation for the change in chemical potential of anhydrous NaBr, valid for the temperature range 200 to 900 K, was obtained from fitting heat-capacity, enthalpy-change, and density measurements, and is described in Sec. 2. Section 3 gives an estimate of the molar heat capacity for 298.15 K and 0.1 MPa for $NaBr\cdot 2H_2O$. The equation for the changes in chemical potentials with respect to temperature, pressure, and molality for NaBr(aq) was obtained from a global fit to selected values of thermodynamic measurements for the aqueous system. The matrix of experimental values contained measurements of volumetric properties, solvent activities, enthalpy changes, heat capacities, and solubilities from the solid phases. This equation and its agreement with experimental values is described in Sec. 4. Section 5 describes the thermodynamic properties for the dehydration reaction of the dihydrate crystal.

2. Thermodynamic Properties of NaBr(cr)

The equations for the heat capacity of anhydrous NaBr given by Pankratz[2] and by Kelley[3] did not appear to be satisfactory for the purpose of calculating the solubility equilibrium for the present work. Kelley's equation was based on the enthalpy-increment measurements of Magnus,[4] these being the only experimental results available. Pankratz's equation was obtained from a fit to the more recent enthalpy-increment measurements of Gardner and Taylor.[5] Extrapolation of Pankratz's equation to temperatures less than 298.15 K showed a minimum in the heat capacity. The temperature of this minimum was calculated to be 283.4 K. This minimum can be avoided by inclusion of the heat-capacity results of Gardner and Taylor[6] for the temperature region of interest.

In order to obtain an equation for the molar heat capacity of NaBr(cr) valid for the range of temperature of interest in the current work, an equation of the form:

$$C^\circ_{p,\,m,\,NaBr(cr)} = a + bT + cT^{-2} \tag{1}$$

where a, b, and c were adjustable parameters, was fitted to the heat-capacity and enthalpy-increment measurements. The form of Eq. (1) for the enthalpy-increment measurements was:

$$H^\circ_{\mathrm{m},\,T,\,\mathrm{NaBr(cr)}} - H^\circ_{\mathrm{m},\,T_\mathrm{r},\,\mathrm{NaBr(cr)}} = a(T - T_\mathrm{r}) + b(T^2 - T_\mathrm{r}^2)/2 - c(T^{-1} - T_\mathrm{r}^{-1}) \qquad (2)$$

where T and T_r are the upper and lower temperatures of the enthalpy-increment measurement. The heat-capacity results[6] included in the fit spanned the temperature range of 175 to 300 K. The enthalpy-increment results of Gardner and Taylor[5] spanning the temperature range of 374 to 999 K (reference temperature, T_r, = 273.15 K), as well as the four enthalpy-drop results reported by Magnus[4] (reference temperature ≅ 290 K) were also included in the fit.

In order to assess the accuracy of the heat-capacity results of Gardner and Taylor the following comparisons were made. A plot of the difference of Gardner and Taylor's heat-capacity results from those of Berg and Morrison,[7] for NaI(cr), was made. Overlayed on this plot were the differences between Morrison and Patterson's[8] and Ginnings and Furukawa's[9] heat-capacity results for the Calorimetry Conference sample of aluminum oxide; the two sets of Morrison's results were obtained with approximately the same calorimeter. This plot indicated agreement of the three sets within 0.2% to 0.4% from 80 to 255 K. The pattern of the difference of Gardner and Taylor's results from those of Morrison is similar to that of the difference between Ginnings and Furukawa's results and those of Morrison. Birch *et al.*[10] measured the heat capacity of NaBr(cr) for temperatures below 20 K; these values were in good agreement with Gardner and Taylor's heat capacities. It was assumed that the uncertainty of Gardner and Taylor's heat-capacity calorimetric method was 0.2% for the temperature region of the values included in the data fit. The agreement of Birch *et al.*'s and Gardner and Taylor's low-temperature heat capacities, combined with the observation that $S^\circ_{\mathrm{m,\,cr}}$ is only 1.46 J·K^{-1}·mol^{-1} for 20 K,[6] indicates that little significant change of the 298.15 K value for $S^\circ_{\mathrm{m,\,cr}}$ given by Gardner and Taylor (86.82 J·K^{-1}·mol^{-1}) would be obtained from a re-evaluation of the low-temperature heat-capacity results (for example, a one percent difference in the heat-capacity results for temperatures less than 20 K alters the 298.15 K heat-capacity value by 0.02 J·K^{-1}·mol^{-1}, significantly less than the uncertainty in the value). Thus, Gardner and Taylor's value of $S^\circ_{\mathrm{m,\,cr}}$ for 298.15 K was used for the present work.

The temperature dependence of the heat capacities calculated from Gardner and Taylor's enthalpy-increment measurements, as either the average heat capacities or calculated from a fitted equation, e.g. values in Gardner and Taylor's Table 2,[5] did not agree with the temperature dependence of their heat-capacity results. The difference between these two sets of results corresponded to a systematic error of 0.4% in either the enthalpy-increment results or in the heat-capacity results, but not both. An average heat capacity from 372 to 290 K calculated from Magnus' enthalpy-increment results did show good agreement with the temperature dependence of the measured heat capacities. On the basis of this comparison the uncertainty assigned to Magnus' results was 1.0% and that assigned to Gardner and Taylor's enthalpy-increment results was 3%. This latter value was somewhat larger than the actual inaccuracy of their measurements and was chosen in order that the larger number of experimental points did not cause undue skewing of the fitted curve in the region where the more accurate experimental results existed. Weighting factors for Eq. (1) were calculated from these estimates of uncertainty. The least-squares estimated parameters for Eq. (1) are given in Table 1. The weighted residuals from the fit are shown in Fig. 1.

The 0.1 MPa molar volumes of NaBr(cr), from 273.15 to 323.19 K, reported by Baxter and Wallace[11] were fitted with the equation:

$$V^\circ_{\mathrm{m,\,cr},\,p_\mathrm{r}} = d + eT\,. \qquad (3)$$

The parameters d and e are given in Table 1. The compressibility of NaBr(cr) is small in the temperature range of interest here and was not included in the equation for the molar Gibbs energy of the anhydrous crystal.

The equation for the molar Gibbs energy of NaBr(cr) is:

$$G^\circ_{\mathrm{m,\,cr}} = G^\circ_{\mathrm{m,\,cr},\,T_\mathrm{r},p_\mathrm{r}} - (T - T_\mathrm{r})\,S^\circ_{\mathrm{m},\,T_\mathrm{r},\,p_\mathrm{r}} + \int_{T_r}^{T} C^\circ_{p,\,\mathrm{m,\,cr},\,p_\mathrm{r}}\,\mathrm{d}T - T\int_{\mathrm{T_r}}^{T} (C^\circ_{p,\,\mathrm{m,\,cr},\,p_\mathrm{r}}/T)\mathrm{d}T + \int_{\mathrm{p_r}}^{\mathrm{p}} V^\circ_{\mathrm{m,\,cr},\,p_\mathrm{r}}\mathrm{d}p \qquad (4)$$

where T_r and p_r were chosen as 298.15 K and 0.1 MPa. $G^\circ_{\mathrm{m,\,cr},\,T_\mathrm{r},p_\mathrm{r}}$ is not experimentally accessible. The thermodynamic properties for formation ($\Delta_\mathrm{f}G^\circ_\mathrm{m}$, $\Delta_\mathrm{f}H^\circ_\mathrm{m}$) of both NaBr(cr) and NaBr·2H$_2$O (cr) for 298.15 K, 0.1 MPa are discussed in a subsequent section.

TABLE 1. Least-squares estimated parameters for Eqs. (1, 3)

Parameter	Value
a	48.332 J·K^{-1}·mol^{-1}
b	1.3684×10^{-2} J·K^{-2}·mol^{-1}
c	-9.4026×10^{4} J·K·mol^{-1}
d	30.963 cm^3·mol^{-1}
e	3.877×10^{-3} cm^3·K^{-1}·mol^{-1}

3. Thermodynamic Properties of NaBr·2H$_2$O(cr)

There are few accurate measurements of the thermodynamic properties of NaBr·2H$_2$O(cr). A value for $C_{p,\,\mathrm{m,\,NaBr\cdot2H_2O(cr)}}$ for 298.15 K, 0.1 MPa was estimated to be 138 J·K^{-1}·mol^{-1} by combining the value of $C^\circ_{p,\,m,\,\mathrm{cr}}$ for NaBr(cr) with 87 J·K^{-1}·mol^{-1}, an approximate value for

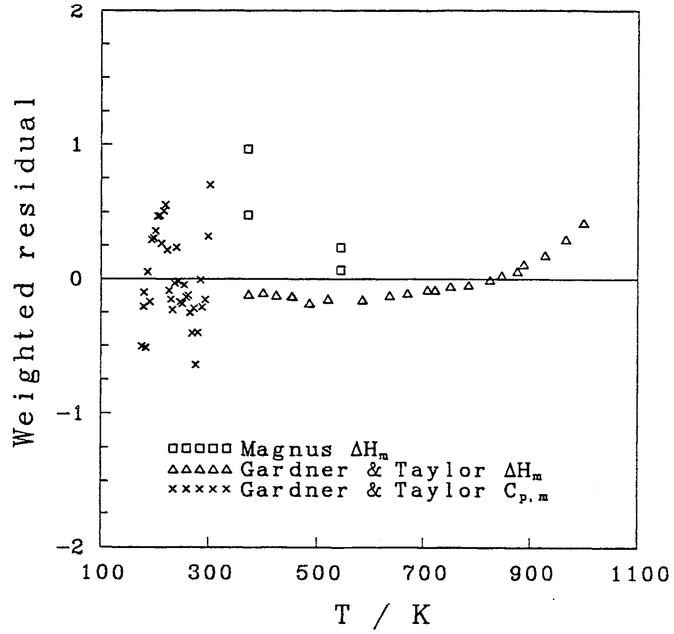

FIG. 1. Weighted residuals from fitting Eq. (1) to the heat-capacity and enthalpy-change measurements for NaBr(cr) against temperature.

the heat capacity contribution for two waters of hydration.

This value was obtained by comparison with other electrolytes. A value for $S^\circ_{m,\ T_r,\ p_r,\ \mathrm{NaBr{\cdot}2H_2O(cr)}}$, was determined from fitting to the experimental solubilities of the dihydrate phase and other thermodynamic results for NaBr(aq).

This result is discussed in detail in a later section.

4. Thermodynamic Properties of NaBr(aq)

4.1. Description of Equations

A modified form of the ion-interaction model of Pitzer[12] was used in the present work to express the excess thermodynamic properties of the solution. Description of Pitzer's equation can be found elsewhere[13] and so only sufficient exposition to allow the use of the present equation is presented here. Pitzer's equation for the excess Gibbs energy per kg of water, n_w, is:

$$\frac{G^{\mathrm{ex}}}{n_w RT} = -4|z_M z_X|A_\phi \ln(1 + bI^{1/2}) + 2\nu_M\nu_X(m^2 B_{\mathrm{MX}} + m^3\nu_M z_M C_{\mathrm{MX}}) \qquad (5)$$

$$B_{\mathrm{MX}} = \beta^{(0)}_{\mathrm{MX}} + 2\beta^{(1)}_{\mathrm{MX}}\,[1 - (1 + \alpha I^{1/2})\exp(-\alpha I^{1/2})]/(\alpha^2 I). \qquad (6)$$

In Eqs. (5, 6), $\beta^{(0)}_{\mathrm{MX}}$, $\beta^{(1)}_{\mathrm{MX}}$, and C_{MX} are adjustable parameters (ion-interaction parameters) that are dependent on temperature and pressure, z_M and z_X are the charges of the cation and the anion, respectively, α and b were chosen to be constants with the values 2.0 $\mathrm{kg^{1/2}{\cdot}mol^{-1/2}}$ and 1.2 $\mathrm{kg^{1/2}{\cdot}mol^{-1/2}}$, respectively, ν_M and ν_X are the stoichiometric numbers of cations and anions formed upon dissociation. A_ϕ is the Debye-Hückel coefficient for the osmotic coefficient.

Occasionally it is found that Eqs. (5, 6) do not give as satisfactory a representation of experimental data as may be desired. In such cases, additional terms of increasing order in molality are often appended to Eq. (5), e.g. $D_{\mathrm{MX}}m^4$, $E_{\mathrm{MX}}m^5$, etc. When the properties of a high-order polynomial are considered, one wonders if these high-order molality functions are always the most useful solution to the problem. In the present work an alternate modification of Pitzer's equation was used.

For the reasons given for the ionic-strength dependence of the second virial coefficient,[12] an ionic-strength dependence of the third virial coefficient is not unexpected. An ionic-strength dependence of the third virial coefficient was assumed for the present work. For simplicity, it was assumed that the functional form of the ionic-strength dependence of the third virial coefficient was similar in nature to that for the second virial coefficient, for the osmotic coefficient. This assumption results in an ionic-strength dependent C_{MX} that is expressed for the present work as:

$$C_{\mathrm{MX}} = C^{(0)}_{\mathrm{MX}} + 4C^{(1)}_{\mathrm{MX}}\,[6-(6+6\alpha_2 I^{1/2}+3\alpha_2^2 I+\alpha_2^3 I^{3/2})\exp(-\alpha_2 I^{1/2})]/(\alpha_2^4 I^2), \qquad (7)$$

where $C^{(0)}_{\mathrm{MX}}$ and $C^{(1)}_{\mathrm{MX}}$ are adjustable parameters, dependent on temperature and pressure. The ionic-strength dependence of the third virial coefficient improves the quality of fit for NaBr(aq), the present work, and also for

NaCl(aq) and Na_2SO_4(aq), as yet unpublished work. For NaCl(aq), optimum values of α_2 were found to be near 2 $kg^{1/2}\cdot mol^{-1/2}$, the same as the value of α in Eq. (6). Thus we take α_2 in Eq. (7), and throughout the remainder of this work, to be the same as α in Eq. (6).

The excess Gibbs energy, G^{ex}, is related to the Gibbs energy of the solution, G, as:

$$G^{ex} = G - n_1 G^{\circ}_{m,1} - n_2 G^{\circ}_{m,2} + RT\nu n_2(1 - \ln m/m^{\circ}) \tag{8}$$

where n_1 and n_2 are the number of moles of solvent and solute, respectively, m is the stoichiometric molality, n is the number of ions formed upon complete dissociation of the electrolyte and m is 1.0 $mol\cdot kg^{-1}$. The standard-state molar Gibbs energy for solvent and solute are $G^{\circ}_{m,1}$ and $G^{\circ}_{m,2}$, respectively. The standard states were chosen to be pure liquid for the solvent and the hypothetical one molal ideal solution for the solute, at the temperature and pressure of interest, rather than at the temperature of interest and an arbitrary pressure. The Debye-Hückel coefficients used in the present work were calculated from the equation of state for water of Hill,[1] the dielectric-constant equation of Archer and Wang,[14] and the definitions given by Bradley and Pitzer.[15]

Appropriate differentiation of Eq. (5) leads to the osmotic coefficient, ϕ, and the stoichiometric activity coefficient, $\gamma_{\pm}$,:

$$\phi - 1 = -|z_M z_X| A_{\phi} \frac{I^{1/2}}{1+bI^{1/2}} + m\frac{2\nu_M\nu_X}{\nu}$$
$$\left(\beta^{(0)}_{MX} + \beta^{(1)}_{MX}\exp)(-\alpha I^{1/2})\right) +$$
$$m^2\frac{4\nu_M{}^2\nu_X}{\nu}\left(C^{(0)}_{MX} + C^{(1)}_{MX}\exp(-\alpha I^{1/2})\right) \tag{9}$$

$$\ln\gamma_{\pm} = -|z_M z_X| A_{\phi}\left(\frac{I^{1/2}}{1+bI^{1/2}} + \frac{2}{b}\ln(1+bI^{1/2})\right) +$$
$$m\frac{2\nu_M\nu_X}{\nu}\left\{2\beta^{(0)}_{MX} + \frac{2\beta^{(1)}_{MX}}{\alpha^2 I}\left[1 - \left(1+\alpha I^{1/2} - \frac{\alpha^2 I}{2}\right)\exp(-\alpha I^{1/2})\right]\right\}$$
$$+ m^2\frac{2\nu_M{}^2\nu_X z_M}{\nu}\left\{3C^{(0)}_{MX} + 4C^{(1)}_{MX}\,[6-(6+6\alpha I^{1/2} + 3\alpha^2 I +\right.$$
$$\left.\alpha^3 I^{3/2} - \alpha^4 I^2/2)\exp(-\alpha I^{1/2})]/(\alpha^4 I^2)\right\}. \tag{10}$$

The relative apparent molar enthalpy, L_{ϕ}, is:

$$L_{\phi} = \nu|z_M z_X| A_H \ln(1 + bI^{1/2})/2b -$$
$$2\nu_M\nu_X RT^2(mB^L_{MX} + m^2\nu_M z_M C^L_{MX}) \tag{11}$$

where:

$$B^L_{MX} = \left(\frac{\partial\beta^{(0)}_{MX}}{\partial T}\right)_p + 2\left(\frac{\partial\beta^{(1)}_{MX}}{\partial T}\right)_p \times$$
$$[1-(1+\alpha I^{1/2})\exp(-\alpha I^{1/2})]/\alpha^2 I \tag{12}$$

$$C^L_{MX} = \left(\frac{\partial C^{(0)}_{MX}}{\partial T}\right)_p + 4\left(\frac{\partial C^{(1)}_{MX}}{\partial T}\right)_p \times$$
$$[6 - (6 + 6\alpha I^{1/2} + 3\alpha^2 I + \alpha^3 I^{3/2})\exp(-\alpha I^{1/2})]/(\alpha^4 I^2) \tag{13}$$

and where A_H is the Debye-Hückel coefficient for apparent molar enthalpy. The constant-pressure apparent molar heat capacity, $C_{p,\phi}$, is:

$$C_{p,\phi} = C^{\circ}_{p,m,2} + \nu|z_M z_X| A_C \ln(1 + bI^{1/2})/2b$$
$$- 2\nu_M\nu_X RT^2(mB^C_{MX} + m^2\nu_M z_M C^C_{MX}) \tag{14}$$

where:

$$B^C_{MX} = \left(\frac{\partial^2\beta^{(0)}_{MX}}{\partial T^2}\right)_p + \frac{2}{T}\left(\frac{\partial\beta^{(0)}_{MX}}{\partial T}\right)_p$$
$$+2\left\{\left(\frac{\partial^2\beta^{(1)}_{MX}}{\partial T^2}\right)_p + \frac{2}{T}\left(\frac{\partial\beta^{(1)}_{MX}}{\partial T}\right)_p\right\} \times$$
$$[1-(1+\alpha I^{1/2})\exp(-\alpha I^{1/2})]/\alpha^2 I \tag{15}$$

$$C^C_{MX} = \left(\frac{\partial^2 C^{(0)}_{MX}}{\partial T^2}\right)_p + \frac{2}{T}\left(\frac{\partial C^{(0)}_{MX}}{\partial T}\right)_p$$
$$+4\left\{\left(\frac{\partial^2 C^{(0)}_{MX}}{\partial T^2}\right)_p + \frac{2}{T}\left(\frac{\partial C^{(0)}_{MX}}{\partial T}\right)_p\right\} \times$$
$$[6-(6+6\alpha I^{1/2} + 3\alpha_2 I + \alpha^3 I^{3/2})\exp(-\alpha I^{1/2})]/(\alpha^4 I^2) \tag{16}$$

and where A_C is the Debye-Hückel coefficient for apparent molar heat capacity and $C^{\circ}_{p,m,2}$ is the standard-state molar heat capacity of the solute. The apparent molar volume of a solution, V_{ϕ}, is:

$$V_{\phi} = V^{\circ}_{m,2} + \nu|z_M z_X| A_V \ln(1 + bI^{1/2})/2b +$$
$$2\nu_M\nu_X RT(mB^V_{MX} + m^2\nu_M z_M C^V_{MX}) \tag{17}$$

where:

$$B^V_{MX} = \left(\frac{\partial\beta^{(0)}_{MX}}{\partial P}\right)_T + 2\left(\frac{\partial\beta^{(1)}_{MX}}{\partial P}\right)_T \times$$
$$[1-(1+\alpha I^{1/2})\exp(-\alpha I^{1/2})]/\alpha^2 I \tag{18}$$

$$C^V_{MX} = \left(\frac{\partial C^{(0)}_{MX}}{\partial p}\right)_T + 4\left(\frac{\partial C^{(1)}_{MX}}{\partial p}\right)_T \times$$
$$[6-(6+6\alpha I^{1/2}+3\alpha^2 I+\alpha^3 I^{3/2})\exp(-\alpha I^{1/2})]/(\alpha^4 I^2) \tag{19}$$

and where A_V is the Debye-Hückel coefficient for apparent molar volume and $V^{\circ}_{m,2}$ is the standard-state volume of the solute.

In order to avoid the complex temperature and pressure behavior of $V^{\circ}_{m,2}$ and $C^{\circ}_{p,m,2}$, Eqs. (17, 14) were rewritten, following, in part, the example of Rogers and Pitzer.[16] The analogous equation for a reference molality was subtracted from the appropriate equation for the molality of interest to obtain, in the case of V_{ϕ},

$$V_{\phi} = V_{\phi,m_r} + \nu|z_M z_X| A_V \ln\{(1 + bI^{1/2})/(1+bI_r{}^{1/2})\}/2b$$
$$+2\nu_M\nu_X RT\{(m - m_r)B^V_{MX} + (m^2 - m_r{}^2)\nu_M z_M C^V_{MX}\} \tag{20}$$

where m_r is the chosen reference molality and I_r, V_{ϕ,m_r}

are the ionic strength and the apparent molar volume that correspond to m_r, respectively. $V_{\phi,\,m_r}$ has a less extreme temperature and pressure dependence than does $V^{\circ}_{m,\,2}$, however, this temperature and pressure dependence may be reduced further by rewriting Eq. (20) as:

$$V_{\phi} + \upsilon_w/n_r = V(m_r)/n_r + \nu|z_M z_X|A_V \ln\{(1+bI^{1/2})/(1+bI_r^{1/2})\}/2b + 2\nu_M\nu_X RT\{(m-m_r)B^V_{MX} + (m^2-m_r^2)\nu_M z_M C^V_{MX}\} \qquad (21)$$

where υ_w is the volume of 1 kg of water, $V(m_r)$ is the volume of a quantity of solution of molality m_r which contains 1 kg of water and n_r is the number of moles of solute in this quantity of solution. This rearrangement requires the definition of the apparent molar property, which is:

$$X_{\phi} = \frac{X - n_1 X^{\circ}_{m,\,1}}{n_2} \qquad (22)$$

where X is the measured property for a quantity of solution containing n_1 moles of solvent and n_2 moles of solute. $X(m_r)$ is the desired slowly changing function, if m_r is chosen to be sufficiently large. In the present work m_r was chosen to be 6 mol·kg^{-1}. Equations similar to Eq. (21) may be written for the other apparent molar properties. The analogous equation for apparent molar heat capacity is:

$$C_{p,\,\phi} + c_{p,\,w}/n_r = C_p(m_r)/n_r + \nu|z_M z_X|A_C \ln\{(1+bI^{1/2})/(1+bI_r^{1/2})\}/2b - 2\nu_M\nu_X RT^2\{(m-m_r)B^C_{MX} + (m^2-m_r^2)\nu_M z_M C^C_{MX}) \qquad (23)$$

where $C_p(m_r)$ is the heat capacity of a quantity of solution containing one kg of solvent at the desired temperature and pressure and $c_{p,\,w}$ is the heat capacity of one kg of water. The pressure dependence of $C_p(m_r)/n_r$ is contained in $V(m_r)/n_r$ and so the only additional variable parameters introduced were those which described the behavior of $C_p(m_r)/n_r$ along an isobar. This isobar was chosen to be 0.1 MPa; other choices had little effect on the overall quality of fit. $C_p(m_r)/n_r$ along this 0.1 MPa isobar will be referred to as $C_{p,\,p_r}(m_r)/n_r$

The partial molar Gibbs energy of the solute in its standard state at temperature T and pressure p, $G^{\circ}_{m,\,2,\,T,p}$, may be written in terms of the above equations as:

$$G^{\circ}_{m,\,2\,T,p}, = G^{\circ}_{m,\,2\,T_r,p_r} + \frac{n_1 G^{\circ}_{m,\,1,\,T_r,p_r} - n_1 G^{\circ}_{m,\,1,\,T,p}}{n_r} + \frac{G^{ex}_{T_r,\,p_r,\,m_r} - G^{ex}_{T,\,p,\,m_r}}{n_r} - (T-T_r)\left(S^{\circ}_{2,\,m,\,T_r,\,P_r} + \frac{n_1 S^{\circ}_{1,\,m,\,T_r,\,P_r}}{n_r} + \frac{S^{ex}_{T_r,p_r,m_r}}{n_r}\right) - T\int_{T_r}^{T}\frac{1}{T^2}\int_{T_r}^{T} C_{p,\,p_r}(m_r)/n_r\,dT\,dT + \int_{p_r}^{p} V(m_r)/n_r\,dp \qquad (24)$$

where:

$$S^{ex}_{T_r,\,p_r} = -\left(\frac{\partial G^{ex}_{T_r,\,p_r}}{\partial T}\right)_p . \qquad (25)$$

T_r and p_r were chosen to be 298.15 K and 0.1 MPa, respectively. The values of $S^{\circ}_{1,\,m,\,T_r,\,P_r}$ and $S^{\circ}_{2,\,m,\,T_r,\,P_r}$ were taken from Cox *et al.*[17] to be 69.95 and 141.0 J·K^{-1}·mol^{-1}, respectively. Cox *et al.*'s value for $S^{\circ}_{2,\,m,\,T_r,\,P_r}$ for NaBr(aq) was obtained from a global fit to available data for several aqueous electrolytes, with the parameters being the thermodynamic properties of the individual ions. Thus, the Cox *et al.* value for $S^{\circ}_{2,\,m,\,T_r,\,P_r}$ was considered immutable for the present work.

The equations describing the solubility of the anhydrous and dihydrate solid phases are:

$$\Delta_{sol}G^{\circ}_{anhydrous} = G^{\circ}_{m,\,2} - G^{\circ}_{m,\,cr,\,anhydrous} = -2RT\ln(m_s\gamma_{\pm,\,s}) \qquad (26)$$

and

$$\Delta_{sol}G^{\circ}_{dihydrate} = G^{\circ}_{m,\,2} + 2G^{\circ}_{m,\,1} - G^{\circ}_{m,\,cr,\,dihydrate} = -2RT\ln(m_s\gamma_{\pm,\,s}) - 2RT\ln a_{w,\,s}\,. \qquad (27)$$

where $G^{\circ}_{m,2}$, $G^{\circ}_{m,\,1}$, and $G^{\circ}_{m,cr,i}$ are the molar Gibbs energies for the solute, the pure liquid, and the *i*th crystal phase all at a given T and p, respectively, $\Delta_{sol}G^{\circ}_i$ is the standard-state molar Gibbs energy for the solution process of the *i*th crystal phase and m_s, $\gamma_{\pm,\,s}$ and $a_{w,\,s}$ are the saturation molality, the mean stoichiometric activity coefficient for the solute at saturation, and the activity of water for the saturation molality, respectively. Of course, $G^{\circ}_{m,\,2}$, $G^{\circ}_{m,\,1}$ and $G^{\circ}_{m,\,cr,\,i}$ cannot be evaluated and so Eqs. (26, 27) were rewritten as:

$$\Delta_{sol}G^{\circ}_{anhydrous,\,T} = \Delta_{sol}G^{\circ}_{anhydrous,\,T_r} + \{G^{\circ}_{m,\,2,\,T} - G^{\circ}_{m,\,2,\,T_r}\} - \{G^{\circ}_{m,\,cr,\,anhydrous,\,T} - G^{\circ}_{m,\,cr,\,anhydrous,\,T_r}\} = -2RT\ln(m_s\gamma_{\pm,\,s}) \quad (28)$$

and

$$\Delta_{sol}G^{\circ}_{dihydrate,\,T} = \Delta_{sol}G^{\circ}_{dihydrate,\,T_r} + \{G^{\circ}_{m,\,2,\,T} - G^{\circ}_{m,\,2,\,T_r}\} - \{G^{\circ}_{m,\,cr,\,dihydrate,\,T} - G^{\circ}_{m,\,cr,\,dihydrate,\,T_r}\} + 2\{G^{\circ}_{m,\,1,\,T} - G^{\circ}_{m,\,1},\,T_r\} = -2RT\ln(m_s\gamma_{\pm,\,s}) - 2RT\ln a_{w,\,s} \qquad (29)$$

The first braced term of Eqs. (28, 29) was obtained from Eq. (24), the second braced term of Eq. (28) was obtained from Eq. (4), the third braced term of Eq. (29) was obtained from the equation of Hill.[1] The second braced term of Eq. (29) was expressed as:

$$\{G^{\circ}_{m,\,cr,\,dihydrate,\,T} - G^{\circ}_{m,\,cr,\,dihydrate,\,T_r}\} = -(T-T_r)\,S^{\circ}_{m,\,cr,\,dihydrate,\,T_r,\,p_r} + 138\ \text{J·K}^{-1}\text{·mol}^{-1}\{(T-T_r) - T\ln(T/T_r)\} \qquad (30)$$

Solubility measurements were included in the global data fit. The two Gibbs energies of solution at the reference temperature, T_r, and reference pressure, p_r, were treated as adjustable parameters, as was $S^{\circ}_{m,\,cr,\,dihydrate,\,T_r,p_r}$. In addition, the experimental solubility results contribute to the determination of the parameters for the excess Gibbs energy for the solution through Eq. (24).

For the dehydration reaction :

$$NaBr{\cdot}2H_2O(cr) = NaBr(cr) + 2H_2O(g)\,, \qquad (31)$$

the Gibbs energy of reaction for 298.15 K and 0.1 MPa, per mole of H_2O, is:

$$\Delta_{\mathrm{dec}}G_{\mathrm{m},\,T_r,\,p_r} =$$

$$(\Delta_f G^{\circ}_{\mathrm{anhydrous},\,T_r,\,p_r} + 2\Delta_f G^{\circ}_{\mathrm{H_2O(g)},\,T_r,\,p_r} - \Delta_f G^{\circ}_{\mathrm{dihydrate},\,T_r,\,p_r})/2 \quad (32)$$

where $\Delta_f G^{\circ}_{\mathrm{anhydrous},\,T_r,\,p_r}$ and $\Delta_f G^{\circ}_{\mathrm{dihydrate},\,T_r,\,p_r}$ are the standard-state Gibbs energies of formation of the anhydrous and dihydrate sodium bromide phases at T_r and p_r. The standard-state Gibbs energy of formation of H_2O at T_r and p_r, $\Delta_f G_{\mathrm{H_2O(g)},\,T_r,\,p_r}$, was taken from Cox *et al*. At any given temperature, the Gibbs energy of decomposition, $\Delta_{\mathrm{dec}}G_{\mathrm{m},\,T,\,p_r}$, is :

$$\begin{aligned}\Delta_{\mathrm{dec}}G_{\mathrm{m},\,T,\,p_r} &= \Delta_{\mathrm{dec}}G_{\mathrm{m},\,T_r,\,p_r} + (S^{\circ}_{\mathrm{m,\,H_2O(g)},\,T_r,\,p_r} + \\ &\quad 0.5S^{\circ}_{\mathrm{m,\,anhydrous},\,T_r,\,p_r} - 0.5S^{\circ}_{\mathrm{m,\,dihydrate},\,T_r,\,p_r})(T_r - T) + \\ &\quad \int_{T_r}^{T} (C^{\circ}_{p,\,\mathrm{m,\,H_2O(g)},\,p_r} + 0.5C^{\circ}_{p,\,\mathrm{m,\,anhydrous},\,p_r} - 0.5C^{\circ}_{p,\,\mathrm{m,\,dihydrate},\,p_r})\mathrm{d}T \\ &\quad - T\int_{T_r}^{T} (C^{\circ}_{p,\,\mathrm{m,\,H_2O(g)},\,p_r} + 0.5C^{\circ}_{p,\,\mathrm{m,\,anhydrous},\,p_r} - \\ &\quad 0.5C^{\circ}_{p,\,\mathrm{m,\,dihydrate},\,p_r}) / T\,\mathrm{d}T), \end{aligned} \quad (33)$$

again per mole of water. The heat capacities and entropies for Eq. (33) have been referred to previously. The vapor pressures of water over the dihydrate solid, from 283.15 to 323.75 K were converted to fugacities and included in the global data fit.

Marshall and coauthors[18] have demonstrated the advantage of representing the equilibrium constant for ion association for supercritical temperatures as a function of both solvent density and temperature. Archer[19] extended this approach to temperatures below the solvent critical temperature by representing the excess properties for HCl(aq) for temperatures from ambient to near-critical with an equilibrium model, in which the equilibrium constant was expressed as a function of temperature and solvent density. Subsequently, Holmes *et al.*[20] adapted this approach to the ion-interaction equation in their representation of the experimental results for HCl(aq) by means of an ion-interaction equation in which the parameters were given as a function of solvent density and temperature. The experimental results considered by Holmes *et al.* for HCl(aq) did not include much volumetric data, other than those which were, in principle, derivable from the pressure dependence of their enthalpies of dilution. The present work expands on this approach.

A significantly larger range of experimental results that defined the pressure dependence of the excess Gibbs energy existed for NaBr(aq) than for HCl(aq) and so the present case provides a better test of the effectiveness of describing the ion-interaction parameters as functions of temperature and solvent density. The ion-interaction parameters for the excess Gibbs energy for NaBr(aq) were expressed as:

$$\begin{aligned}\beta^{(0)}_{\mathrm{MX}} = {} & [b_{1,1} + b_{1,2}(T - T_r)/T^{\circ} + b_{1,3}\{(T - T_r)/T^{\circ}\}^2 + \\ & b_{1,4}T^{\circ}/(T - 225\ \mathrm{K}) + b_{1,5}T^{\circ}/(T - 647\ \mathrm{K}) + b_{1,6}T^{\circ}/T + \\ & b_{1,7}\{T^{\circ}/(T - 225\ \mathrm{K})\}^3 + b_{1,8}\rho/\rho^{\circ} + b_{1,9}\rho T/(\rho^{\circ}T^{\circ}) + \\ & b_{1,10}\rho T^2/(\rho^{\circ}T^{\circ 2}) + b_{1,11}\rho T^{\circ}/\{\rho^{\circ}(T - 225\ \mathrm{K})\} + \\ & b_{1,12}\rho T^{\circ}/(T - 647\ \mathrm{K}) + b_{1,13}\rho^2/\rho^{\circ 2} + \\ & b_{1,14}\rho^2 T/(T^{\circ}\rho^{\circ 2}) + b_{1,15}\rho^2 T^{\circ}/\{\rho^{\circ 2}(T - 225\ \mathrm{K})\} + \\ & b_{1,16}\rho^3/\rho^3]/m^{\circ} \end{aligned} \quad (34)$$

$$\begin{aligned}\beta^{(1)}_{\mathrm{MX}} = {} & [b_{2,1} + b_{2,2}(T - T_r)/T^{\circ} + b_{2,3}\{(T - T_r)/T^{\circ}\}^2 + \\ & b_{2,4}T^{\circ}/(T - 225\ \mathrm{K}) + b_{2,5}T^{\circ}/(T - 647\ \mathrm{K}) + \\ & b_{2,6}T^{\circ}/T + b_{2,7}\{T^{\circ}/(T - 225\ \mathrm{K})\}^3 + b_{2,8}\rho/\rho^{\circ} + \\ & b_{2,9}\rho T/(\rho^{\circ}T^{\circ}) + b_{2,10}\rho T^2/(\rho^{\circ}T^{\circ 2}) + b_{2,11}\rho T^{\circ}/ \\ & \{\rho^{\circ}(T - 225\ \mathrm{K})\} + b_{2,12}\rho T^{\circ}/(T - 647\ \mathrm{K}) + b_{2,13}\rho^2/\rho^{\circ 2} + \\ & b_{2,14}\rho^2 T/(T^{\circ}\rho^{\circ 2}) + b_{2,15}\rho^2 T^{\circ}/\{\rho^{\circ 2}(T - 225\ \mathrm{K})\} + \\ & b_{2,16}\rho^3/\rho^{\circ 3}]/m^{\circ} \end{aligned} \quad (35)$$

$$\begin{aligned}C^{(0)}_{\mathrm{MX}} = {} & [b_{3,1} + b_{3,2}(T - T_r)/T + b_{3,3}\{(T - T_r)/T^{\circ}\}^2 + \\ & b_{3,4}T^{\circ}/(T - 225\ \mathrm{K}) + b_{3,5}T^{\circ}/(T - 647\ \mathrm{K}) + \\ & b_{3,6}T^{\circ}/T + b_{3,7}\{T^{\circ}/(T - 225\ \mathrm{K})\}^3 + b_{3,8}\rho/\rho^{\circ} + \\ & b_{3.9}\rho T/(\rho^{\circ}T^{\circ}) + b_{3.10}\rho T^2/(\rho^{\circ}T^{\circ 2}) + b_{3.11}\rho T^{\circ}/ \\ & \{\rho^{\circ}(T - 225\ \mathrm{K})\} + b_{3,12}\rho T^{\circ}/(T - 647\ \mathrm{K}) + \\ & b_{3,13}\rho^2/\rho^{\circ 2} + b_{3,14}\rho^2 T/(T^{\circ}\rho^{\circ 2}) + b_{3,15}\rho^2 T^{\circ}/ \\ & \{\rho^{\circ 2}(T - 225\ \mathrm{K})\} + b_{3,16}\rho^3/\rho^{\circ 3}]/m \end{aligned} \quad (36)$$

$$\begin{aligned}C^{(1)}_{\mathrm{MX}} = {} & [b_{4,1} + b_{4,2}(T - T_r)/T^{\circ} + b_{4,3}\{(T - T_r)/T^{\circ}\}^2 + \\ & b_{4,4}T^{\circ}/(T - 225\ \mathrm{K}) + b_{4,5}T^{\circ}/(T - 647\ \mathrm{K}) + \\ & b_{4,6}T^{\circ}/T + b_{4,7}\{T^{\circ}/(T - 225\ \mathrm{K})\}^3 + b_{4,8}\rho/\rho^{\circ} + \\ & b_{4,9}\rho T/(\rho^{\circ}T^{\circ}) + b_{4,10}\rho T^2/(\rho^{\circ}T^{\circ 2}) + b_{4,11}\rho T^{\circ}/ \\ & \{\rho^{\circ}(T - 225\ \mathrm{K})\} + b_{4,12}\rho T^{\circ}/(T - 647\ \mathrm{K}) + \\ & b_{4,13}\rho^2/\rho^{\circ 2} + b_{4,14}\rho^2 T/(T^{\circ}\rho^{\circ 2}) + b_{4,15}\rho^2 T^{\circ}/ \\ & \{\rho^{\circ 2}(T - 225\ \mathrm{K})\} + b_{4,16}\rho^3/\rho^{\circ 3}]/m \end{aligned} \quad (37)$$

where T is 1.0 K, ρ° is 1.0 $\mathrm{g{\cdot}cm^{-3}}$ and m is 1.0 $\mathrm{mol{\cdot}kg^{-1}}$. $V(m_r)/n_r$ and $C_p(m_r)/n_r$ were taken as functions of T and p as:

$$\begin{aligned}V(m_r)/n_r = {} & [b_{5,1} + b_{5,2}p/p^{\circ} + b_{5,3}T/(300\ T^{\circ}) + \\ & b_{5,4}(p/p^{\circ})^2 + b_{5,5}\{T/(300\ T^{\circ})\}^2 + b_{5,6}pT/ \\ & (p^{\circ}300T^{\circ}) + b_{5,7}pT^2/\{p^{\circ}(300\ T^{\circ})^2\} + \\ & b_{5,8}p^2 T/(p^{\circ 2}300T) + b_{5,9}\{T/(300T^{\circ})\}^3 + \\ & b_{5,10}\{Tp/(300T^{\circ}p^{\circ}\}^2]V^{\circ} \end{aligned} \quad (38)$$

$$\begin{aligned}C_p(m_r)/n_r = {} & [b_{6,1} + b_{6,2}T/T^{\circ} + b_{6,3}(T/T^{\circ})^2 + \\ & b_{6,4}(T^{\circ}/T) - 2b_{5,5}(p - p_r)T/(p^{\circ}300^2 T^{\circ}) - \\ & b_{5,7}T(p^2 - p_r^2)/(p^{\circ 2}300^2 T^{\circ}) - 6b_{5,9}(T/T^{\circ})^2 \\ & (p - p_r)/(p^{\circ}300^3) - 2b_{5,10}(T/T^{\circ})(p^3 - p_r^3)/ \\ & (3p^{\circ}300^2)]C_p^{\circ} \end{aligned} \quad (39)$$

where V° is 1.0 $\mathrm{cm^3{\cdot}mol^{-1}}$, C_p° is 1.0 $\mathrm{kJ{\cdot}mol^{-1}{\cdot}K^{-1}}$, p° is 1.0 MPa. The functions of Eqs. (34–39) were scaled so that all of the least-squares estimated parameters would be of the same order of magnitude.

The least-squares estimated parameters, $b_{i,j}$, are found in Table 2. The absence of a value for a particular $b_{i,j}$ from Table 2 indicates that it was not used in the final least-squares procedure. The equation for the partial molar Gibbs energy of the solute has explicit variables T, p, and ρ.

4.2. Agreement with Experimental Results for NaBr(aq)

Reported experimental results were reduced to forms which were a compromise between values that were as close to the actually measured experimental quantity as possible and convenience. This reduction was used so as to remove the influence of changes in the properties of water on the input data set (i.e. the effect of a water property on the calculation of an apparent molar property, the effect of a water property on calibration of an instrument, etc.) and to simplify the weighting of experimental results. At the time the least-squares procedure was executed these experimental values were converted into the appropriate quantity for fitting and a weighting factor was calculated from the expected experimental error for the actual measurement. As an example, consider the case of experimental density results obtained with a pycnometer. A pycnometer is calibrated with a fluid of known density; in the case of aqueous solutions the choice of calibrating fluid is usually water. Rather than record the reported values of either the apparent molar volume or the density of the solution, the value of the density of solution divided by the density of water (ρ_w as reported by the original investigator), ρ_s/ρ_w, was stored in the data base. (Simple rearrangement of the equations used for both the calibration of the pycnometric vessel and the subsequent determination of the solution density shows that the quantity ρ_s/ρ_w is the direct result of the experimental observations, i.e. the weighings.) The fitting program calculated the apparent molar volume from the value of ρ_s/ρ_w using the ρ_w calculated from the chosen equation of state for water. The experimental uncertainty in apparent molar volume was also calculated from the expected uncertainty in ρ_s/ρ_w. In this way, the value to be fitted was free from uncertainties due to the difference in the investigators'choice of water density and that calculated from the presently chosen equation of state for water, as well as the change in definition of the liter and changes in atomic weights.

TABLE 2. Least-squares estimated parameters for Eqs. (28–30, 34–39)

Parameter	Value	Parameter	Value	Parameter	Value[a]
$b_{1,1}$	1.71530582184808	$b_{2,1}$		$b_{3,1}$	$-5.10439487733469\times10^{-2}$
$b_{1,2}$	$-1.73252346455901\times10^{-3}$	$b_{2,2}$	$6.91694564546029\times10^{-3}$	$b_{3,2}$	$5.43671292746595\times10^{-5}$
$b_{1,3}$		$b_{2,3}$	$-2.36002542074249\times10^{-6}$	$b_{3,3}$	
$b_{1,4}$	$-7.12047951860816\times10^{1}$	$b_{2,4}$		$b_{3,4}$	5.85950490319896
$b_{1,5}$		$b_{2,5}$		$b_{3,5}$	
$b_{1,6}$	$-1.06149855919480\times10^{2}$	$b_{2,6}$		$b_{3,6}$	2.67503166447214
$b_{1,7}$		$b_{2,7}$	$-4.32670425215971\times10^{-3}$	$b_{3,7}$	
$b_{1,8}$	-3.17819715551732	$b_{2,8}$	2.08920730994785	$b_{3,8}$	$4.74961164927853\times10^{-4}$
$b_{1,9}$		$b_{2,9}$	$-5.94507937562393\times10^{-3}$	$b_{3,9}$	
$b_{1,10}$	$1.11014863667444\times10^{-6}$	$b_{2,10}$		$b_{3,10}$	
$b_{1,11}$	$1.03396881250985\times10^{2}$	$b_{2,11}$		$b_{3,11}$	-8.25906888284215
$b_{1,12}$	-5.03344509639110	$b_{2,12}$		$b_{3,12}$	$3.38335601272359\times10^{-1}$
$b_{1,13}$	2.92477266480196	$b_{2,13}$		$b_{3,13}$	
$b_{1,14}$		$b_{2,14}$		$b_{3,14}$	$-3.43893892665741\times10^{-5}$
$b_{1,15}$	$-3.48635153871965\times10^{1}$	$b_{2,15}$		$b_{3,15}$	2.55121785563878
$b_{1,16}$	$-10.1862025333775\times10^{-1}$	$b_{2,16}$		$b_{3,16}$	
$b_{4,1}$		$b_{5,1}$	$1.74722236351206\times10^{-1}$	$\Delta_{\mathrm{sol}}G^{\circ}_{\mathrm{anhydrous},\,T_r,p_r}$	-17.006 ± 0.029 kJ·mol^{-1}
$b_{4,2}$		$b_{5,2}$	$-1.05498649133375\times10^{-4}$	$\Delta_{\mathrm{sol}}G^{\circ}_{\mathrm{dihydrate},\,T_r,p_r}$	-11.881 ± 0.022 kJ·mol^{-1}
$b_{4,3}$	$4.49429821594186\times10^{-7}$	$b_{5,2}$	$1.68973227859952\times10^{-2}$	$S^{\circ}_{m,\,\mathrm{cr,\,dihydrate},Tr,\,p_r}$	177.66 ± 0.5 J·K^{-1}·mol^{-1}
$b_{4,4}$	-1.98475043408448	$b_{5,4}$			
$b_{4,5}$	$1.14947024443337\times10^{1}$	$b_{5,5}$	$-2.38299260480859\times10^{-3}$		
$b_{4,6}$	$-4.15575163219869\times10^{1}$	$b_{5,6}$	$1.28774220130067\times10^{-4}$		
$b_{4,7}$	$2.98484853131687\times10^{3}$	$b_{5,7}$	$-7.83136107954372\times10^{-5}$		
$b_{4,8}$		$b_{5,8}$			
$b_{4,9}$		$b_{5,9}$	$5.58947543213706\times10^{-3}$		
$b_{4,10}$		$b_{5,10}$	$4.77254889781834\times10^{-8}$		
$b_{4,11}$		$b_{6,1}$	2.02845536497279		
$b_{4,12}$		$b_{6,2}$	$-3.87815647610758\times10^{-3}$		
$b_{4,13}$		$b_{6,3}$	$3.68379636925015\times10^{-6}$		
$b_{4,14}$		$b_{6,4}$	$-1.37650520324255\times10^{2}$		
$b_{4,15}$		T_r	298.15 K		
$b_{4,16}$		p_r	0.1 MPa		

[a] The ± values are 95% confidence intervals within the global data representation.

water, as well as the change in definition of the liter and changes in atomic weights.

With occasional exceptions, weighting factors were defined as the inverse of the square of the expected error in the measurement $(1/\sigma_{exp})^2$. Exceptions to this are described in the text. Explanations of the differences of the experimental uncertainties used in this work from those described by the investigators are described in the text.

4.2.1. Volumetric Properties

Volumetric results included in the data representation for NaBr(aq) spanned the temperature and pressure ranges of 273.15 to 623.15 K and from near the vapor pressure of water to 150 MPa. A list of the volumetric results considered for the global data fit is given in Table 3.

Samples of NaBr obtained from chemical-supply houses usually contain some small amount of chloride impurity. The chloride impurity cannot be removed by recrystallization from water. Indeed, recrystallization from water increases the concentration of chloride in the precipitate.[42] Gibson and Loeffler[35] showed that repeated recrystallization of NaBr from water created significant errors in the observed density of concentrated solutions and that this error became larger with each recrystallization. They also showed that repeated recrystallization of NaBr from aqueous hydrobromic acid yielded a sample of NaBr of which the density of aqueous solutions did not change with repeated recrystallization. Despite these results, some of the literature references to density measurements described their NaBr(cr) as having been repeatedly recrystallized from water. When all other things were equal, experimental volumetric results obtained from recrystallized samples of NaBr(cr) were given significantly smaller weights for the least-squares procedure.

The reported experimental volumetric measurements for NaBr(aq) were classified in one of five different categories. Pycnometric and other results in which a calibration with a single reference fluid (water) was performed

TABLE 3. Literature sources for the volumetric properties of NaBr(aq)

Ref.	Temperatire Range (K)	Pressure Range[a] (MPa)	Molality Range ($mol\cdot kg^{-1}$)	n	Type	σ_{est}[b]	σ_{fit}
21	298.15	0.1	m_s	2	ρ_s/ρ_w	550×10^{-6}	1243×10^{-6} [c]
22	298.15	0.1	0.006 – 1.0	9	ρ_s/ρ_w	40×10^{-6}	18×10^{-6} [d]
23	298.15	0.1	0.16 – 6.65	40	$\Delta_{dil}V_\phi$	0.05–0.015	0.014 [e]
24	298.15	0.1	0.1 – 0.47	6	ρ_s/ρ_w	50×10^{-6}	19×10^{-6} [c]
25	298.15	0.1	0.06 – 0.54	10	$\rho_s-\rho_w$	5×10^{-6}, 0.1%	38×10^{-6} [f]
26	298.15	0.1	0.05 – 1.8	15	V_ϕ	0.1 – 0.02	0.026 [g]
27	298.15	0.1	0.6 – 4.0	3	$\rho_s-\rho_w$	5×10^{-6}, 0.1%	17×10^{-6} [f]
28	298.15	0.1	0.68 – 8.38	6	ρ_s/ρ_w	400×10^{-6}	518×10^{-6} [c]
29	298.15	0.1	0.1 – 1.0	10	$\rho_s-\rho_w$	5×10^{-6}, 0.1%	24×10^{-6} [f]
30	298.15	0.1	0.35 – 4.36	8	ρ_s	400×10^{-6}	192×10^{-6} [c]
31	298.15	0.1	1.0 – 8.34	9	$\rho_s-\rho_w$	U	4100×10^{-6} [c]
32	273.15 – 343.34	0.1	0.28 – 6.65	20	ρ_s/ρ_w	40×10^{-6}	118×10^{-6} [c]
33	273.15 – 348.59	0.1	m_s	10	ρ_s/ρ_w	1.0×10^{-3}	1.3×10^{-3} [c]
34	298.15 – 318.15	0.1	1.2 – 5.2	10	ρ_s/ρ_w	40×10^{-6}	76×10^{-6} [h]
35,36	298.15 – 358.15	0.1 – 100	0.5 – 7.74	175	ρ_s/ρ_w	40×10^{-6}	53×10^{-6} [c]
37	298 – 623	** – 150	0.20 – 7.95	429	ν_s	$3-5\times10^{-3}$	3.9×10^{-3} [i]
38	293.15 – 363.15	0.1	0.10 – 6.48	36	ρ_s	$0.2 - 2.0\times10^{-3}$	0.64×10^{-3} [c]
39	288.15 – 328.15	0.1	0.05 – 8.0	81	ρ_s/ρ_w	0.1%	215×10^{-6} [j]
40	298.15	0.1 – 40	0.05 – 4.97	40	$\rho_s-\rho_w$	U	799×10^{-6} [c]
41	321.7 – 549.8	** – 32	0.05 – 3.03	174	$\rho_s-\rho_w$	[k]	511×10^{-6} [c]

[a] ** indicates that the lowest pressure for the data set changed with the experimental temperature.

[b] The letter U indicates that these points were given an insignificant weight in the least-squares procedure.

[c] Units are $g\cdot cm^{-3}$.

[d] Units are $g\cdot cm^{-3}$. Lowest molality point was given an insignificant weight in the least-squares procedure, it has been included in σ_{fit}.

[e] Units are $cm^3\cdot mol^{-1}$. Dilutions from 6.65 $mol\cdot kg^{-1}$ $\sigma_{exp} = 0.05$ $cm^3\cdot mol^{-1}$, dilutions from 2.11 and 1.84 $mol\cdot kg^{-1}$ $\sigma_{exp} = 0.015$ $cm^3\cdot mol^{-1}$, dilutions from 1.22 $mol\cdot kg^{-1}$ $\sigma_{exp} = 0.018$ $cm^3\cdot mol^{-1}$.

[f] Units are $g\cdot cm^{-3}$. Data were weighted as the larger of 5×10^{-6} $cm^3\cdot mol^{-1}$ or 0.1% of $\rho_s-\rho_w$.

[g] Units are $cm^3\cdot mol^{-1}$. Expected uncertainties ranged from 0.1 $cm^3\cdot mol^{-1}$ for 0.05 $mol\cdot kg^{-1}$ to 0.02 $cm^3\cdot mol^{-1}$ for 0.6 $mol\cdot kg^{-1}$ and larger.

[h] Units are $g\cdot cm^{-3}$, lowest molality for 298.15 K given an insignificant weight in the least-squares procedure, σ_{fit} does not contain the residual for this point.

[i] Units are $cm^3\cdot g^{-1}$. Results for temperatures less than 373.15 K $\sigma_{exp} = 3000\times10^{-6}$ $cm^3\cdot g^{-1}$, $\sigma_{exp} = 5000\times10^{-6}$ $cm^3\cdot g^{-1}$ for temperatures greater than 373.15 K.

[j] Units are $g\cdot cm^{-3}$. Data were weighted as $\sigma_{exp} = 0.1\%$ of $\rho_s-\rho_w$.

[k] Weighted according to the σ_{exp} given in Ref. 41.

were recorded as the ratio of solution density to water density, ρ_s/ρ_w, where the water density value was that reported as having been used in the calibration of the apparatus. Vibrating-tube densimeter and magnetic-float densimeter results were used as the difference in density between solution and water, $\rho_s-\rho_w$. Vibrating-tube densimeters require a calibration with two reference fluids of known densities and so are not as amenable to reduction as pycnometric results. Results from vibrating-tube densimeters, including those designed for operation at near-ambient conditions, are subject to systematic errors in the calibration constant. These errors appear to be dependent on the choice of calibrating fluid. For example, a figure in the operating manual for the Sodev densimeter[43] shows calibration constants obtained with different reference fluids; the calibration constants varied by approximately 0.1%. Another possible source of systematic error in results obtained from vibrating-tube densimeters may arise from adsorption of solute on the walls of the densimeter tube. Indications of adsorption effects for vibrating-tube densimeters, as well as methods which may be used to correct for such effects, have been reported by Archer *et al.*[44] for aqueous surfactants and by Majer *et al.*[45] for aqueous electrolytes. Thus, the potentially lower accuracy of these instruments, for concentrated solutions, does not warrant reduction of these values for water calibration errors. Values obtained by means of a dilatometer are the change in volume for a given change in concentration and were described as $\Delta_{dil}V_\phi$. These values were treated in the same way as enthalpy of dilution values, $\Delta_{dil}L_\phi$. Values of V_ϕ and ρ_s for which insufficient information existed with which to reduce these values to their experimentally measured quantities were recorded as such. These values were usually, but not always, given lesser weight for the least-squares procedure.

Figure 2 shows the difference between V_ϕ calculated from the fitted equation and values reported in the literature or calculated from volumetric measurements reported in the literature for 298.15 K and 0.1 MPa. The $\rho_s-\rho_w$ values of Grzybowski and Atkinson[31] showed very

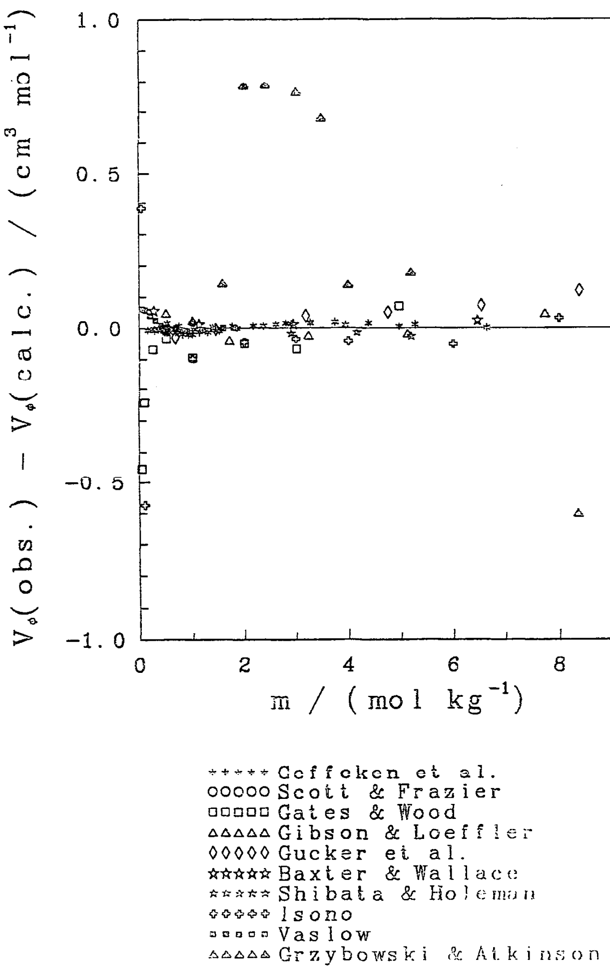

FIG. 2. Residuals, in terms of apparent molar volume, for 298.15 K and 0.1 MPa against the square root of molality.

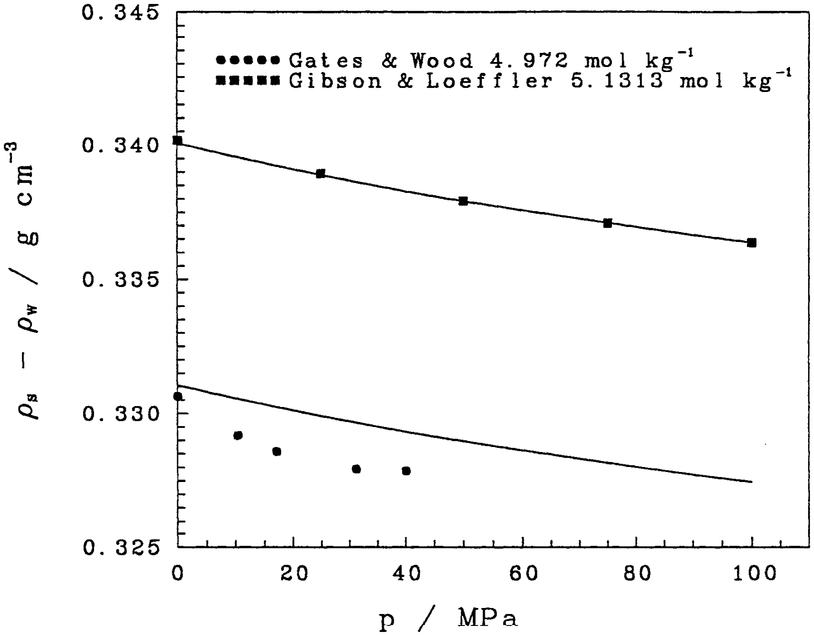

FIG. 3. Comparison of values of difference in density between solution and water, $\rho_s - \rho_w$, against pressure for 298.15 K The solid lines were calculated from the global fit.

large disagreement with the other values and thus were given no significant weight in the least-squares procedure. It is also noted that not all of the V_ϕ values given by Grzybowski and Atkinson could be calculated from their reported values of $\rho_s - \rho_w$, the difference being as large as 9 cm^3·mol^{-1} in one case. Grzybowski and Atkinson did not discuss the disagreement of their values with the earlier literature values.

Figure 3 shows $\rho_s - \rho_w$ for 4.972 mol·kg^{-1} NaBr(aq) reported by Gates and Wood[40] and values calculated for 5.131 mol·kg^{-1} NaBr(aq) from the ρ_s/ρ_w of Gibson and Loeffler,[36] both for 298.15 K. The pressure dependence of Gates and Wood's $\rho_s - \rho_w$ was somewhat different from that of Gibson and Loeffler's measurements. For 0.101 MPa, Gates and Wood's values agreed with the remainder of the literature values within their experimental uncertainties. Differences occurred for increasing molality and pressures greater than 10 MPa; the largest difference was approximately four to five times larger than Gates and Wood's estimated uncertainty. Because other experimental results exist for the region of conditions considered by Gates and Wood, their results were given an insignificant weight in the least-squares procedure.

The root-mean-square (r.m.s.) error for Majer *et al.*'s[41] results was 511×10^{-6} g·cm^{-3}. In the region of temperature in which there was an overlap of the results of Majer *et al.* with those of Gibson and Loeffler[36], there also appeared to be a systematic difference for pressures significantly removed from ambient. The average weighted error for some of Majer's sets of measurements were: −0.005 for 321.7 K and 0.8 MPa; −1.6 for 321.7 K and 32.2 MPa; −1.47 for 347.6 K and 0.8 MPa; and −3.3 for 347.6 K and 32.5 MPa. These values[a] showed that there existed a discrepancy of the pressure dependence of Majer's results from those of Gibson and Loeffler's and that the sign of this discrepancy was the same as that observed for the difference between Gates and Wood's[40] values from Gibson and Loeffler's. Additionally, the value of this difference was approximately the same for both sets and not strongly dependent on temperature between 298 and 358 K. The densimeter used by Majer *et al.* was similar to that of Gates and Wood. Majer's densimeter was calibrated with H_2O, D_2O, and occasionally N_2, whereas Gates and Wood used H_2O and N_2. Both methods of calibrating did not detect this 0.4% discrepancy in the pressure dependence of the calibrations and so the difference between the vibrating-tube densimeter results and those from the compression apparatus was perplexing. Similar differences were not found for NaCl(aq). Although there existed this difference for NaBr(aq), it must be observed that it was a percentage error in $\rho_s - \rho_w$, not in ρ_s, and so for low concentrations the vibrating-tube apparatus still yielded $\rho_s - \rho_w$ results which were orders of magnitude more accurate than those obtained with conventional high-temperature *PVT* methods. The r.m.s. error for

---

[a] (Crudely speaking, the average weighted error should be zero if the source of error is random and the sample is sufficiently large, a nonzero value between 1 and −1 is indicative of a systematic error that falls within the estimated standard error of the measurements, absolute values of the average weighted error larger than 1 indicate a systematic error larger than the estimated standard error of the measurements.)

Egorov *et al.*'s results was 3900×10^{-6} g·cm^{-3}, which was within their stated uncertainties.

There does not exist a thermodynamic relation between the speed of sound in a solution and the isentropic compressibility, β_S. If absorption of the propagated wave is small for the selected frequency and other uncertainties are also small,[102] then the isentropic compressibility can be approximated as:

$$\beta_S = \frac{1}{u^2\,\rho_s} \tag{40}$$

where u is the speed of sound. The isentropic compressibility is related to the isothermal compressibility, β, as:

$$\beta = \beta_S + \frac{\alpha_s^2 T}{\rho_s c_{p,s}} \tag{41}$$

where α_s and $c_{p,s}$ are the expansivity and the specific heat capacity of the solution. Figure 4 shows a comparison of the isentropic compressibility calculated from the fitted equation and that calculated from reported speeds of sound for 298.15 K.[29,31] The values calculated from Millero *et al.*'s results showed an r.m.s. difference from the fitted equation of 1.1×10^{-6} MPa^{-1}. This difference was significantly greater than Millero's estimated uncertainty in β_S of 2×10^{-8} MPa^{-1},[46] however it was satisfactory for the purpose of this work. The difference between Millero *et al.*'s 1.000 mol·kg^{-1} β_S value and Grzybowski and Atkinson's 1.000 mol·kg^{-1} β_S value was approximately 2.0×10^{-6} MPa^{-1} , which was also significantly greater than 2×10^{-8} MPa^{-1}. In any case, the largest difference of the isentropic compressibilities calculated from the speed-of-sound measurements from those calculated from the present equation was only 3%. This is an acceptable level of agreement. The value of the apparent molar isentropic compressibility for infinite dilution, $K^{\circ}_{\phi,S}$, for 298.15 K and 0.1 MPa calculated from the fitted equation, -38.4 m^3·mol^{-1}·MPa^{-1} was in reasonable agreement with the literature values of -40.7 m^3·mol^{-1}·MPa^{-1},[47] -41.8 m^3·mol^{-1}·MPa^{-1},[29] -42.8 m^3·mol^{-1}·MPa^{-1},[48] the literature values being uncertain by 2 to 3 m^3·mol^{-1}·MPa^{-1}.[29]

4.2.2. Activity and Thermal Properties

A list of the solute and solvent activity, enthalpy of dilution and heat-capacity data sets considered for the present work is given in Table 4. A significant portion of the available data was excluded from the final least squares fit. Most of these sets were excluded because of incompatibilities with the remainder of the data sets.

It has not been possible to create an accurate and reversible sodium metal electrode for use in aqueous systems and thus the most reliably measured solute activity coefficients for NaBr(aq) were those obtained by means of bromide concentration cells. Concentration-cell measurements yield the ratio of activity coefficients of two solutions, one for each concentration. Concentration-cell results were thus stored in the data base as the ratio of the two activity coefficients, γ_2/γ_1. The logarithm of γ_2/γ_1 was treated in the least-squares procedure as the difference in the logarithms of the activity coefficients for the two molalities. Harned's[50] and Harned and Crawford's[51] measurements appeared to be the most accurate of these results. Tanner and Lamb[71] reported differences of the

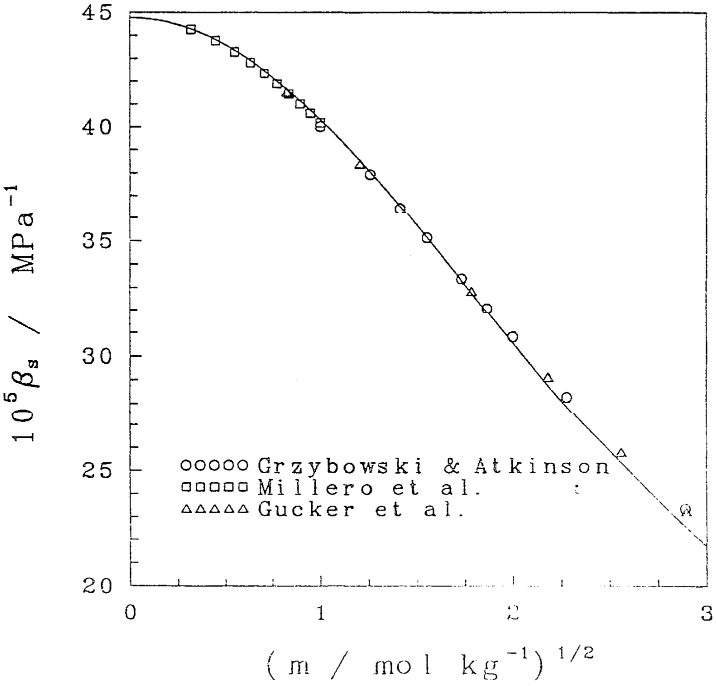

FIG. 4. The isentropic compressibility calculated from the fitted equation compared with that estimated from measurements of the speed of sound in NaBr(aq) for 298.15 K and 0.1 MPa.

concentration dependence of their measured heat capacities from values calculated from the second temperature derivative of Harned and Crawford's activity coefficients. This discrepancy was large enough to cause difficulties in fitting to the thermal data for the present work. The following procedure was used to determine which of these two data sets was in error. The 0.1 MPa $C_{p,\phi}$ of Tanner and Lamb were fitted with an equation which represented their results with an r.m.s. difference of 1.3 $J{\cdot}K^{-1}{\cdot}mol^{-1}$. Values of $C_{p,\phi}$ were interpolated for the temperatures and molalities of the 17.5 MPa $C_{p,\phi}$ results reported by White *et al.*[72] These two sets of values were differenced to obtain a set of $\Delta C_{p,\phi}$(obs.) for the pressure change of 0.1 to 17.5 MPa. The volumetric results described above were fitted with only the pressure dependent parameters of Eqs. (34–38). From this fit the $\Delta C_{p,\phi}$(calc.) corresponding to the $\Delta C_{p,\phi}$(obs.) were calculated as:

$$\Delta C_{p,\phi}(\text{calc.}) = \int_{p_2}^{p_1} -T\left(\frac{\partial^2 V_\phi}{\partial T^2}\right)_p dp. \tag{42}$$

TABLE 4. Literature sources for the activity and thermal properties of NaBr(aq)

Ref.	Temperature Range (K)	Pressure Range[a] (MPa)	Molality Range (mol·kg⁻¹)	n	Type[b]	ρ_{est}[c]	σ_{fit}
49	298.15	0.1	0.03 – 3.02	9	$\ln(\gamma_2/\gamma_1)$	U	0.0074
50	298.15	0.1	0.2 – 4.0	9	$\ln(\gamma_2/\gamma_1)$	U	0.0065
51	273.15 – 313.15	0.1	0.2 – 4.0	108	$\ln(\gamma_2/\gamma_1)$	0.02	0.0086
52	298.15	0.1	0.005 – 0.2	6	$\ln(\gamma_\pm)$	U	0.016
53	T_{fus}	0.1	0.003 – 1.20	31	$\Delta_{\text{fus}}T$	[d]	0.0045[e]
54	T_{fus}	0.1	0.03 – 1.47	26	$\Delta_{\text{fus}}T$	[d]	0.0034[e]
55	298.15	-	0.12 – 3.99	33	ϕ	0.006	0.0036[e]
56	298.15	-	m_s	1	ϕ	0.010	0.017[e]
57	298.15	-	2.8 – 8.9	16	ϕ	U	0.017[e]
58	298.15	-	3.0 – 9.17	14	ϕ	0.006	0.0027[e]
59	298.15	-	1.9 – 4.2	5	ϕ	0.003	0.0030[e]
60	298.15	-	2.7 – 5.4	5	ϕ	0.003	0.0029[e]
61	298.15	-	0.1 – 9.13	23	$p_s - p_w$	U	0.052[e]
62	293.4 – 353.15	-	m_s	6	$p_s - p_w$	U	0.046[e]
63	272.7 – 356.9	-	2.0 – 7.0	46	$p_s - p_w$	ϕ	0.0064[e]
64	423.15 – 573.15	-	0.72 – 8.69	32	$p_s - p_w$	U	0.067[e]
65	298.15	0.1	0.0002 – 0.1	35	$\Delta_{\text{dil}}L_\phi$	0.004	0.005[g]
66	298.15	0.1	0.0017 – 9.004	9	$\Delta_{\text{dil}}L_\phi$	0.030	0.019[g]
67	298.15	0.1	0.9 – 1.5	23	$\Delta_{\text{dil}}L_\phi$	0.002	0.0007[g]
68	298.15	0.1	0.15 – 3.0	10	$\Delta_{\text{dil}}L_\phi$	0.030	0.023[g]
69	303.15	0.1	0.26 – 1.08	7	$\Delta_{\text{dil}}L_\phi$	0.005	0.005[g]
70	373.15	0.2	0.03 – 8.0	8	$\Delta_{\text{dil}}L_\phi$	0.010 – 0.020	0.023[g]
70	423.15	0.5	0.03 – 8.0	11	$\Delta_{\text{dil}}L_\phi$	0.020 – 0.030	0.028[g]
70	473.15	1.6	0.03 – 8.0	9	$\Delta_{\text{dil}}L_\phi$	0.030	0.078[g]
71	298.15	0.1	0.05 – 1.0	7	$C_{p,\phi}$	0.012	0.0044[g]
27	298.15	0.1	0.028 – 1.0	17	$C_{p,\phi}$	0.004	0.0017[h]
72	278.15 – 358.15	0.1	0.09 – 7.6	40	$C_{p,\phi}$	0.006 – 0.003	0.0018[i]
73	306.15 – 350.30	17.0 – 17.5	0.05 – 3.0	66	$c_{p,s}/c_{p,w}$	[j]	0.0079[h]
73	400.92 – 500.9	17.0 – 17.5	0.05 – 3.0	72	$c_{p,s}/c_{p,w}$	[j]	0.0085[h]
73	551.90 – 602.74	17.0 – 17.5	0.05 – 3.0	59	$c_{p,s}/c_{p,w}$	[j]	0.119[k]
74	283.15 – 323.75	-	-	18	p_{dec}	0.013	0.017[l]
74	283.15 – 373.15	-	m_s	13	$p_s - p_w$	[m]	0.021[e]

[a] – indicates that the pressures for the data set changed with the experimental conditions.

[b] The symbol $p_s - p_w$. refers to the difference in vapor pressure between solution and solvent, p_{dec} is the vapor pressure of water in equilibrium with $NaBr{\cdot}2H_2O$.

[c] The letter U indicates that these points were given an insignificant weight in the least-squares procedure.

[d] Values of σ_{exp} were calculated as the uncertainty in osmotic coefficient due to an uncertainty of 0.003 K for Ref. 53, or the uncertainties given for Ref. 54, respectively, or 0.003, whichever was larger.

[e] σ_i in terms of osmotic coefficient.

[f] Values of σ_{exp} were calculated as the uncertainty in osmotic coefficeint due to an uncertainty of 3×10^{-6} MPa or 0.005, whichever was larger

[g] Units are $kJ{\cdot}mol^{-1}$.

[h] Units are $kJ{\cdot}K^{-1}{\cdot}mol^{-1}$.

[i] Units are $kJ{\cdot}K^{-1}{\cdot}mol^{-1}$. These values were assigned weighting factors based on 0.3 of σ_{exp}.

[j] Values of σ_{exp} were calculated from the uncertainties given in Ref. 73; these values vary with temperature and molality, σ_{fit} are given in terms of apparent molar heat capacity, $kJ{\cdot}K^{-1}{\cdot}mol^{-1}$.

[k] Units are $kJ{\cdot}K^{-1}{\cdot}mol^{-1}$. The three values for 577.87 K and 0.0498 $mol{\cdot}kg^{-1}$ were not included in the fit or in σ_{fit}.

[l] Units are kPa.

[m] The vapor pressures of saturated solutions at 10 K intervals, and at 298.15 K, were taken from Ref. 74. Iterations were performed to arrive at a set of saturation molalities corresponding to these temperatures. Values of σ_{exp} were calculated from Ref. 74's estimated uncertainties of pressure of 0.013 kPa for $T \leq$ 348.15 K and 0.13 kPa for $T >$ 348.15 K. The weighted r.m.s. deviation for this data set was 1.3.

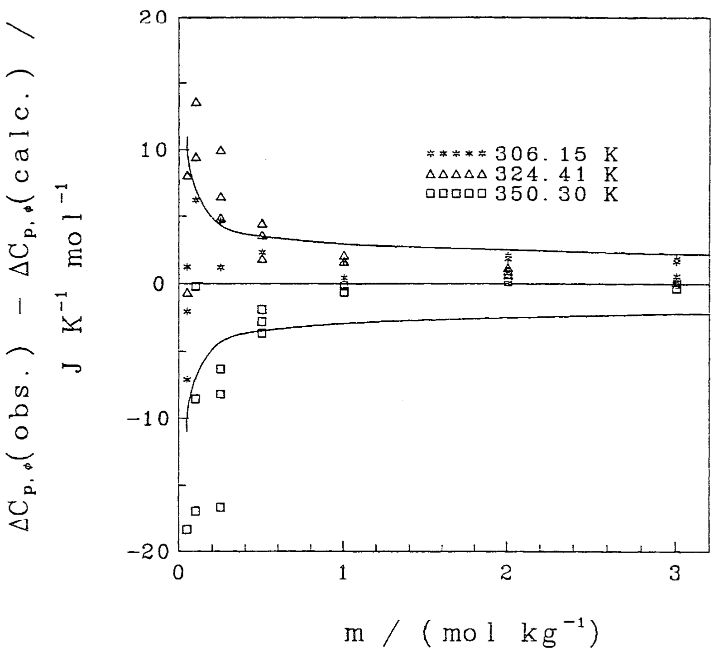

FIG. 5. Difference between the experimentally observed change in apparent molar heat capacity for a 17.5 MPa change in pressure and that calculated form an equation fitted to the experimental volumetric results. The lines are the error estimates of White *et al.*

Figure 5 shows that the calculated pressure dependence of $C_{p,\phi}$ agreed with the experimentally observed behavior within the estimated uncertainties of the White *et al.* results, at least for molalities greater than 0.5 mol·kg^{-1}. White *et al.* measured the ratio of heat capacity of solution to that of water in their mass-flow calorimeter, whereas Tanner and Lamb measured the heat-capacity ratio of two batch calorimeters (vapor space corrections having been applied). In order for the experimental $\Delta C_{p,\phi}$ to have agreed as well as it did with the $\Delta C_{p,\phi}$ calculated from the volumetric fit, either the systematic errors in both sets of heat-capacity results were smaller than ±2 to 3 J·K^{-1}·mol^{-1}, or the systematic errors from these two different calorimeters agreed within ±2 to 3 J·K^{-1}·mol^{-1} and thus cancelled each other in the subtraction. Because the latter of these two choices seemed the more unlikely, the heat capacity data were treated as though they had the experimental uncertainties estimated by the authors and the data of Harned,[50] and Harned and Douglas[49] were given an insignificant weight in the fit to the data. The σ_{exp} for Harned and Crawford's $\ln(\gamma_2/\gamma_1)$ values was given a value 0.02. Figure 6 shows the systematic difference between the globally fitted equation and the 4.0 mol·kg^{-1} activity coefficient results of Harned and Crawford vs. temperature. This difference is seen to be not unrealistically large in both the figure and in the r.m.s. deviation from the fitted equation, as given in Table 4. The experimental results of Lebed *et al.*[52] were obviously inaccurate and given an insignificant weight in the least-squares process.

Values of the solvent activity coefficient for the presently considered results consisted of measurements of the freezing-point depression, solvent vapor pressure, and isopiestic molalities. Values of the osmotic coefficient were calculated from the freezing-point depression, $\Delta_{\text{fus}}T$, as:[75]

$$\phi = -\frac{\left(\dfrac{\Delta_{\text{fus}}H^\circ\,\Delta_{\text{fus}}T}{RT_f^2} + \dfrac{B_1\Delta_{\text{fus}}T^2}{2} + \dfrac{C_1\Delta_{\text{fus}}T^3}{3} + \dfrac{D_1\Delta_{\text{fus}}T^4}{4}\right)}{\nu m M_1} \tag{43}$$

where

$$B_1 = \frac{2\Delta_{\text{fus}}H^\circ}{RT_f^3} - \frac{\Gamma_0}{RT_f^2};\ C_1 = \frac{3\Delta_{\text{fus}}H^\circ}{RT_f^4} - \frac{2\Gamma_0}{RT_f^3} + \frac{\Gamma_1}{2RT_f^2};$$
$$D_1 = \frac{4\Delta_{\text{fus}}H^\circ}{RT_f^5} - \frac{3\Gamma_0}{RT_f^4} + \frac{\Gamma_1}{2RT_f^3} - \frac{\Gamma_2}{3RT_f^2} \tag{44}$$

Craft and Van Hook[75] give $\Delta_{\text{fus}}H^\circ = -6008$ J·mol^{-1}, $\Gamma_0 = -37.7514$ J·K^{-1}·mol^{-1}, $\Gamma_1 = 0.224781$ J·K^{-2}·mol^{-1}, $\Gamma_2 = -1.45867\times10^{-5}$ J·K^{-3}·mol^{-1}. Osmotic coefficients were calculated from the difference in vapor pressure between the solution and the solvent as:[76]

$$\phi = \frac{(G^\circ_{m,1,g} - G^\circ_{m,1})}{RT\nu m M_1} \tag{45}$$

where the difference in chemical potentials for the vapor and the liquid at the temperature and pressure of the solution, $G^\circ_{\text{m},1,g} - G^\circ_{\text{m},1}$, was calculated from the equation of state for water. Because the vapor pressure of the solution can be several MPa less than the vapor pressure of the solvent (e.g. $T > 500$ K), Eq. (45) entailed the use of the equation of state for conditions of T and p substantially outside of the equilibrium region for liquid water.

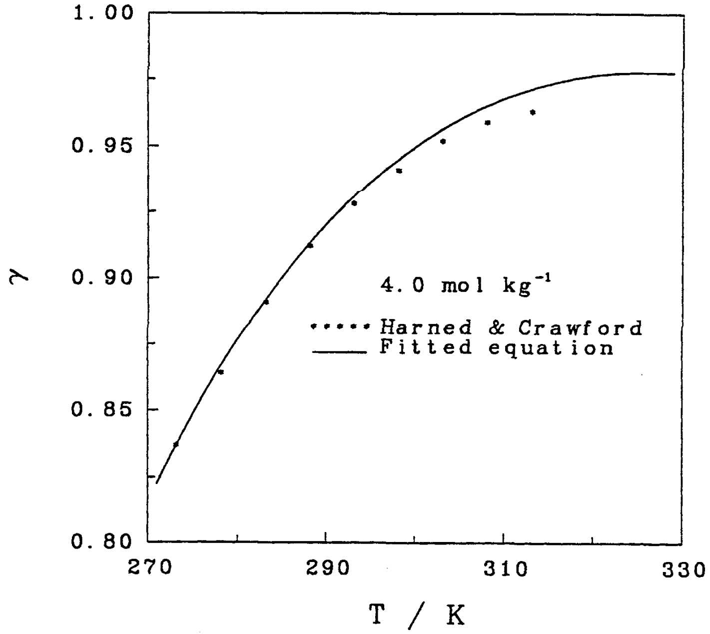

FIG. 6. Comparison of values of the activity coefficient calculated from the fitted equation and the values of Harned and Owen for 4 mol·kg^{-1} NaBr(aq) against temperature.

For 623 K, the values of the properties of water corresponding to pressures for some of the NaBr solutions measured by Mashovets *et al.*[64] could not be calculated with Hill's[1] equation of state.

Osmotic coefficients for Robinson's[55] isopiestic molalities of NaBr(aq) and KCl(aq) and Covington *et al.*'s[59] isopiestic molalities of NaBr(aq) and KCl(aq) were calculated by means of Hamer and Wu's[77] equation for KCl(aq).

Osmotic coefficients for NaCl(aq), the reference solute for Covington *et al.*'s, and Kirgintsev and Luk'yanov's[60] isopiestic molalities, were calculated from Clarke and Glew's[78] equation for NaCl(aq). Osmotic coefficients for Penciner and Marcus'[57] isopiestic molalities of NaBr(aq) and $CaCl_2$(aq) were calculated by means of an equation for $CaCl_2$(aq) reported by Garvin *et al.*[79] Penciner and Marcus' results were given an insignificant weight in the least-squares procedure because their results showed a systematic negative bias from the other osmotic coefficient results. The value of the activity of water for a saturated solution of NaBr for 298.15 K, 0.557 ±0.001, given by Stokes and Robinson was used as given. Their uncertainty for the activity of water for the saturated solution corresponded to an uncertainty of ±0.01 in the osmotic coefficient.

Figure 7 shows the differences between the osmotic coefficients calculated from the freezing-point depressions and the fitted equation. There was a small systematic difference between the results of Damköhler and Weinzerl[54] and those of Scatchard and Prentiss.[53] This difference was approximately the size of the difference of Robinson's[55] and Covington *et al.*'s[59] osmotic coefficients from the fitted equation, for the same molalities. Figure 8 shows the agreement between the fitted equation and the 273.15 and 298.15 K osmotic coefficients. Because of the differences of the freezing point measurements from the 298.15 K results, it is obvious that there will exist systematic differences between the present equation and those based on results for only a single particular temperature, e.g. the equation of Hamer and Wu for NaBr(aq). The residuals for Pearce *et al.*'s[61] observations for large molality extended beyond the upper limit of the figure and approached 0.09 for a molality of 9.0 mol·kg^{-1}. Pearce's results were given no significant weight in the fit. Figure 9 shows a comparison of osmotic coefficients calculated from the vapor-pressure measurements of Jakli and Van Hook.[63] They estimated that values of ϕ calculated from their measurements would be accurate to approximately ±0.01 to ±0.02. Mashovets *et al.*[64] measured the vapor pressure of NaBr solutions for temperatures from 423 to 623 K. These values were also given no significant weight in the determination of the fitted equation. Osmotic coefficients calculated from their results showed some qualitative agreement with the fitted equation for molalities larger than 2−3 mol·kg^{-1} (Fig. 10).

The enthalpies of dilution of Hammerschmid and Robinson,[65] Wallace,[66] Wood *et al.*,[68] and Vaslow,[67] for 298.15 K and 0.1 MPa, as well as the results of Leung and Millero[69] for 303.15 K and 0.1 MPa were all fitted with acceptable r.m.s. deviations. The differences between the fitted equation and Mayrath and Wood's enthalpies of dilution for 373 to 473 K, showed r.m.s. deviations approximately 2.5 times larger than the uncertainties estimated in their work. However, these differences were small when compared to the magnitude of L_ϕ (Fig. 11).

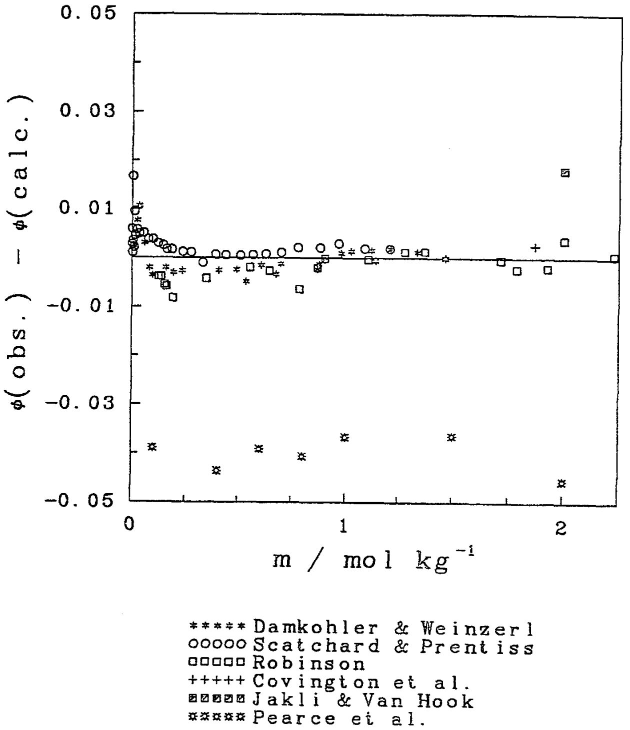

FIG. 7. Residual plot for the osmotic coefficient for temperatures from the freezing point to 298.15 K and from 0 to 2 mol·kg^{-1}.

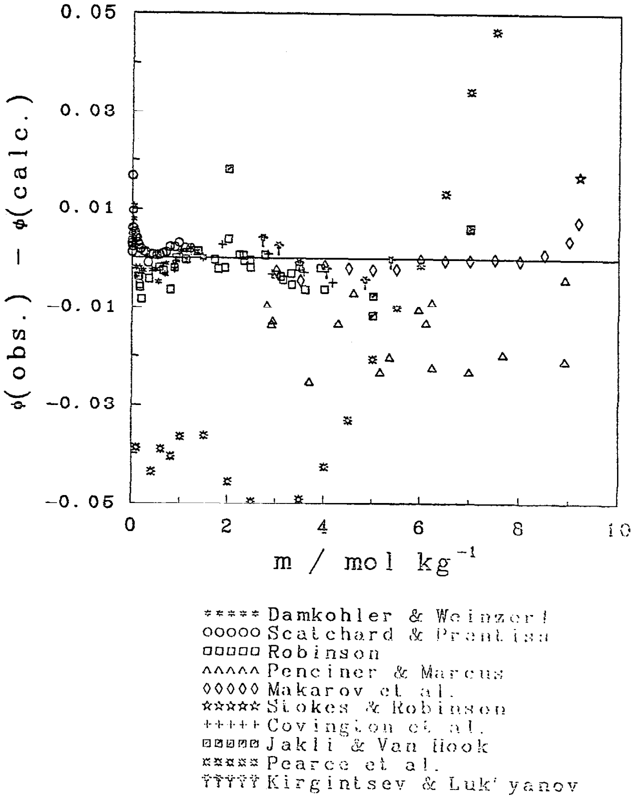

FIG. 8. Residual plot for the osmotic coefficient for temperatures from the freezing point to 298.15 K and from 0 to the saturation molality.

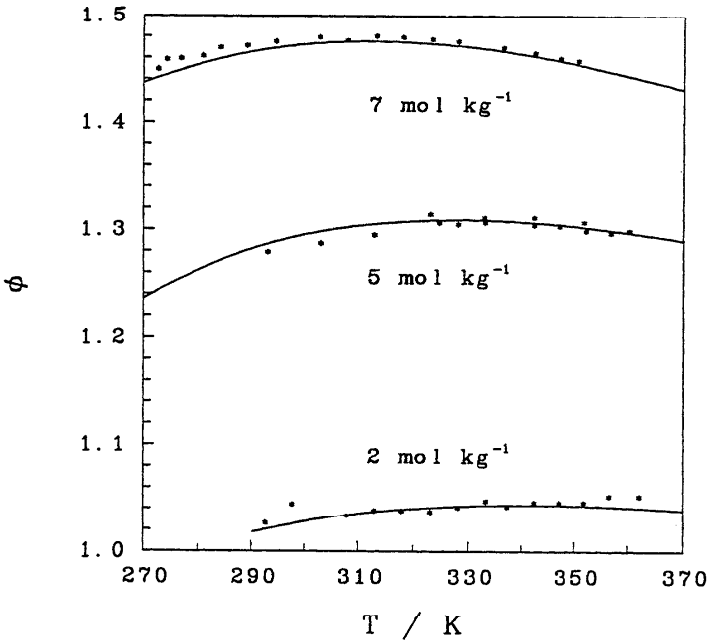

FIG. 9. Comparison of the osmotic coefficients calculated from Jakli and Van Hook's vapor pressure measurements to those calculated from the present equation.

Figures 12–15 show the residuals of $C_{p,\phi}$, from 278 to 602.7 K for the results of Tanner and Lamb,[72] and values calculated from the $c_{p,s}/c_{p,w}$ of White *et al.*[73] Residuals that were systematically biased 2 to 4 times larger than White *et al.*'s expected uncertainties were found for the 577 K data set. There also existed poorer precision in the 577 K results than for temperatures either greater or lesser than 577 K, which suggested the possibility of an experimental difficulty in this particular isothermal data set. The flexibility of the cubic-spline fitting method, used by White *et al.* in their fitting to these results, is such that a greater uncertainty of this one isothermal set of measurements, in a region where $C_{p,\phi}$ was changing rapidly with temperature, might not have been immediately visible. Figure 15 shows a comparison of the $C_{p,\phi}$ calculated from the results of White *et al.*, along with values calculated from the fitted equation, for 1.003 mol·kg^{-1}. It is seen that the difference between the observed values, including those for 577 K, and the fitted function is not great compared to the value of $C_{p,\phi}$.

4.2.3. Solubilities of NaBr·2H$_2$O(cr) and NaBr(cr)

Till this point no experimental results have been described that enabled determination of the two Gibbs energies of solution and the molar entropy of the dihydrate listed in Table 2. In principle, the representations of the experimental results described to this point, when combined with the appropriate reference-temperature Gibbs energies of formation and the standard entropies for each of the species, should be sufficient to calculate the solubilities of the anhydrous and dihydrate solid phases of NaBr as a function of temperature and pressure. Figure 16 shows some of the solubility values given by Linke,[80] and Eddy and Menzies,[81] the latter values having not been included in Linke's compilation. The pressures for these measurements were either 0.1 MPa or the saturation vapor pressure. Values of the solubility calculated from combination of a preliminary representation of the previously described results and the formation properties of Wagman *et al.*[82] are also shown in the figure. It is seen that this combination of values did not provide very accurate calculation of the solubilities. (It is observed that the "Key Values" of Cox *et al.*[17] should not be used in combination with the Wagman *et al.* values for other species, e.g. NaBr(cr), for the purpose of equilibrium calculations. This is because the values for the thermodynamic properties of the species in Ref. 82, which were subsequently revised in Ref. 17, were used in the determination of many of Ref. 82's other species, most of which were calculated from equilibrium observations, such as solubility measurements.)

In some of the preliminary data representations the difference of the calculated solubilities from the observed values were significantly greater for NaBr(cr) than for NaBr·2H$_2$O(cr), near the 0.1 MPa triple-point temperature. This observation implied that it was probably not the solution-property representation which was causing the observed discrepancy with experiment. It was also observed that for the dihydrate solubility, the calculated temperature dependence of the solubility was in error, whereas for the anhydrous solute there was a nearly temperature-independent difference between the observed and calculated values. Examination of the equations

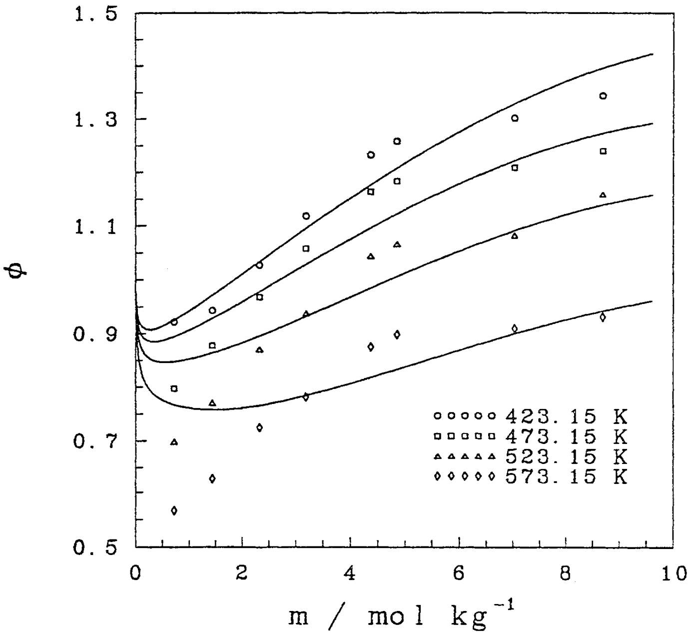

FIG. 10. Values of the osmotic coefficient from 423.15 to 573.15 K and values of the osmotic coefficients calculated from the vapor-pressure measurements of Mashovets *et al.*

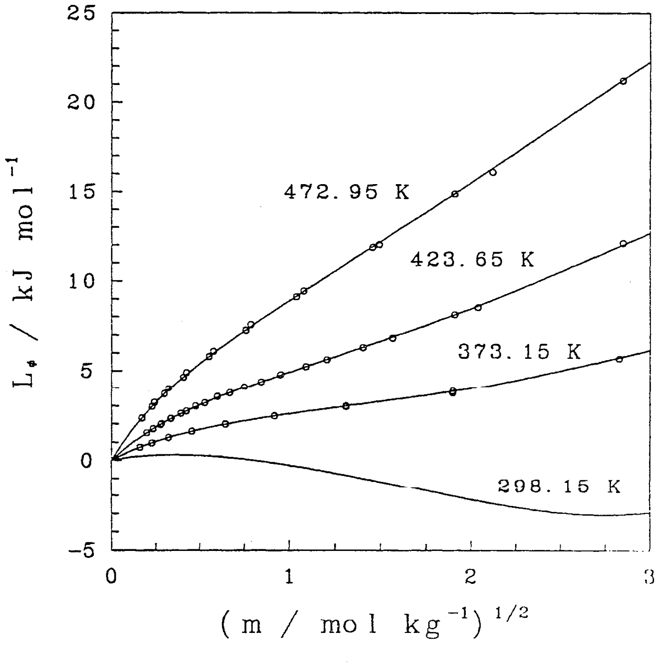

FIG. 11. Comparison of fitted equation with the enthalpy of dilution values of Mayrath and Wood. The enthalpy of dilution values have been plotted as described previously.[96]

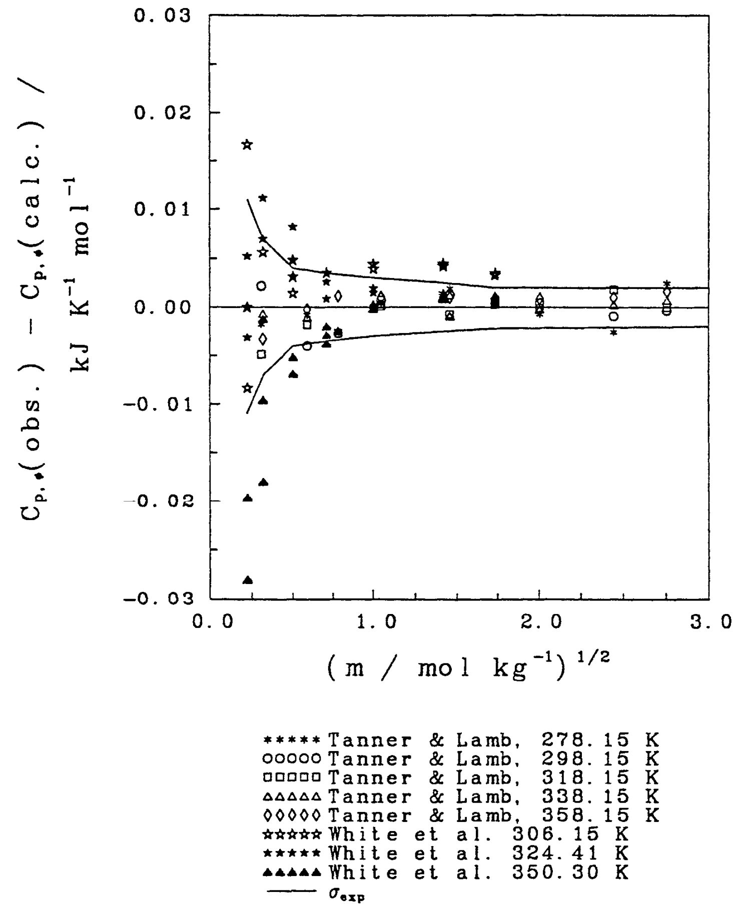

FIG. 12. Residual plot for the fitted heat-capacity measurements for 278.15 to 350.30 K.

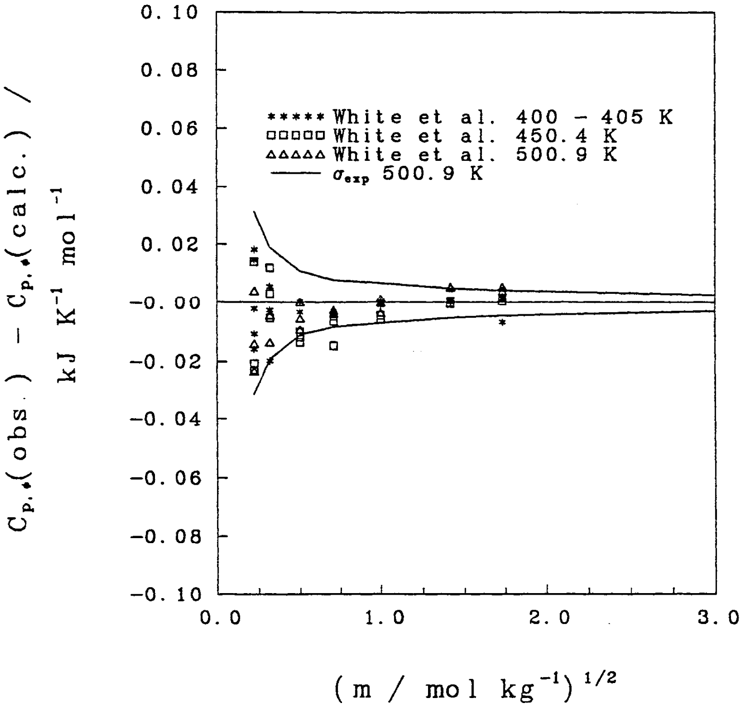

FIG. 13. Residual plot for the fitted heat-capacity measurements for 400 to 501 K.

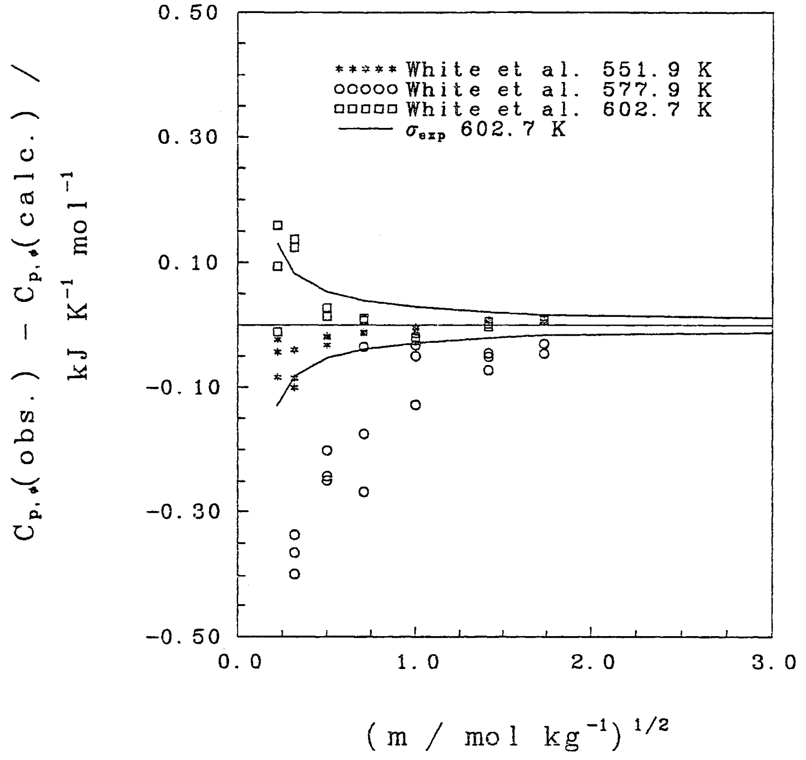

FIG. 14. Residual plot for the fitted heat-capacity measurements for 552 to 603 K.

given above for the dependence of the Gibbs energy of solution on temperature indicated: 1) for the former case, the entropy of the dihydrate phase from Ref. 82 may have been slightly in error; 2) in the latter case, the Gibbs energy of formation of the anhydrous solid phase from Ref. 82 may be in error.

A potential source of these errors can be supposed. In the remainder of this section it is to be realized that the Gibbs energy of formation and/or enthalpy of formation and/or entropy of NaBr(aq) were required for the calculations. For brevity this will not be explicitly stated for each case. Wagman *et al.*'s[82] value for the 298.15 K entropy of the dihydrate phase apparently was obtained from a value for the 298.15 K Gibbs energy of solution for the dihydrate and the value for the enthalpy of solution of the dihydrate recommended by Parker.[83] This Gibbs energy of solution required knowledge of the solute activity coefficient of NaBr(aq), the osmotic coefficient and the saturation molality. The present work indicated that the changes in the solvent activity coefficient sufficient to adjust the solid phase entropy to a value consistent with the temperature dependence of the solubility results were not acceptable in terms of the accuracy of the available measurements. This left the choice of the value for the enthalpy of solution as a possible source of error for the dihydrate entropy.

Wagman *et al.*'s value for the Gibbs energy of formation for the anhydrous crystalline phase, for 298.15 K and 0.1 MPa, apparently was obtained from combination of Gardner and Taylor's[6] value of the 298.15 K entropy with Parker's recommended value for the enthalpy of solution of the anhydrous solid. An uncertainty of 1.1 J·K^{-1}·mol^{-1} in the 298.15 K entropy for NaBr was required to adjust the Gibbs energy of formation to a value which provided reasonably accurate solubilities. The agreement of the enthalpy-drop measurements with the heat-capacity measurements, and the agreement of heat capacities of other substances with the work of others, discussed in Sec. 2, implied that such a large error in the molar entropy was unlikely. Thus, it appeared that the error in Gibbs energy of formation of the anhydrous phase may have arisen in Parker's recommendation of Wallace's[60] value for the enthalpy of solution of NaBr(cr) as the "best" value.

In order to obtain more reliable values for the thermodynamic properties for formation of the two solid phases, solubility measurements from 253.15 K to 523.15 K were incorporated in the least-squares procedure and the two Gibbs energies of solution and the 298.15 K molar entropy of the dihydrate were also included as adjustable parameters in the global data fit. The solubility measurements were given sufficient weight to ensure an accurate representation. The agreement of fitted equation and solubility from 250 to 520 K is shown in Fig. 17. The solubility of NaBr, for temperatures near the upper limits of those depicted in Fig. 17, was outside the region of concentration generally accepted as being within the limits of applicability of the ion-interaction equation used in the present work. Additionally, for the combination of large

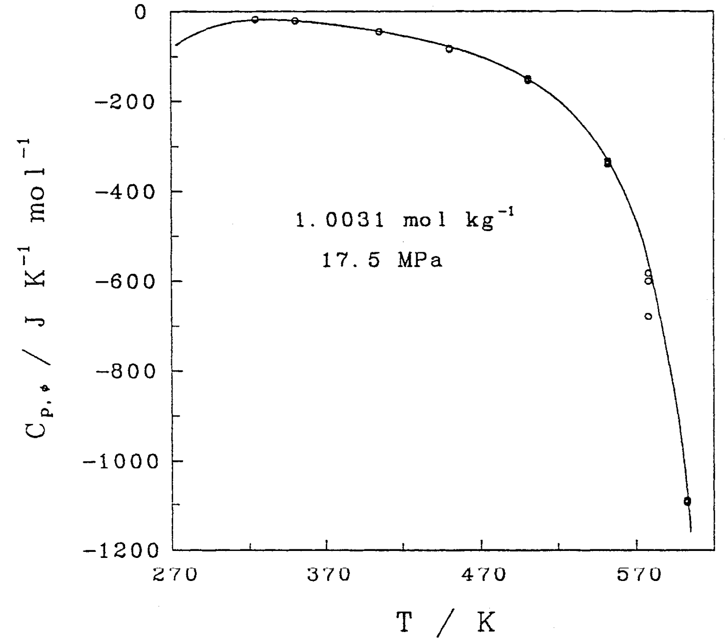

FIG. 15. The apparent molar heat capacity for a 1.0031 mol·kg^{-1} solution, experiment compared to fitted equation.

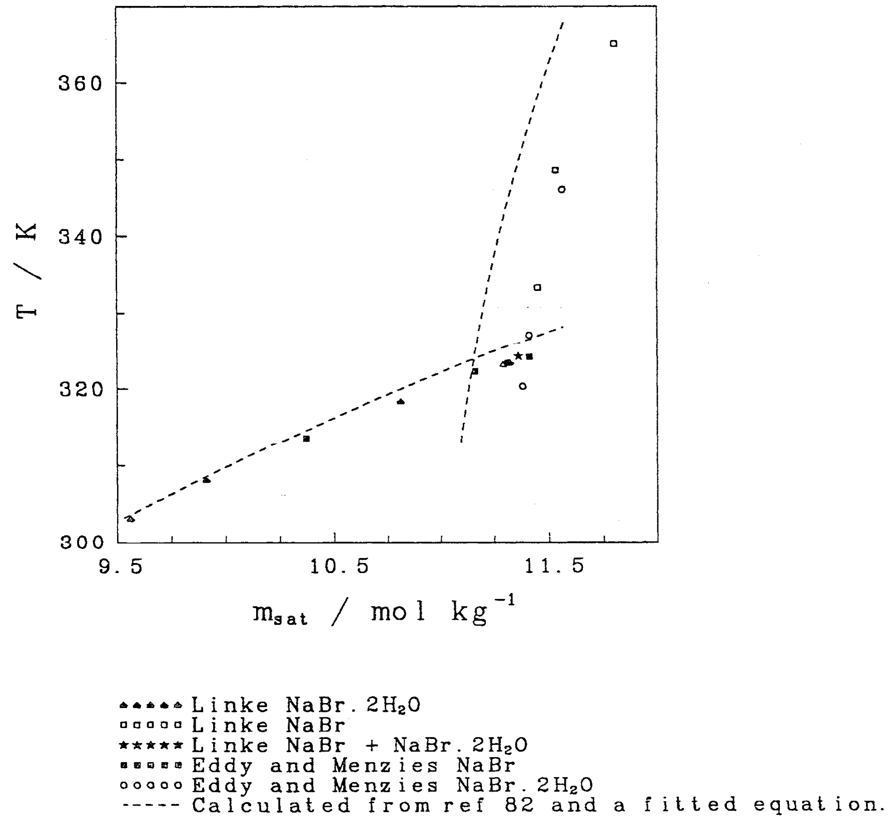

FIG. 16. Values of the solubility of NaBr(cr) and NaBr·2H$_2$O(cr) calculated from the present equation for the solution properties combined with thermodynamic properties of the solid phases from Wagman *et al.*

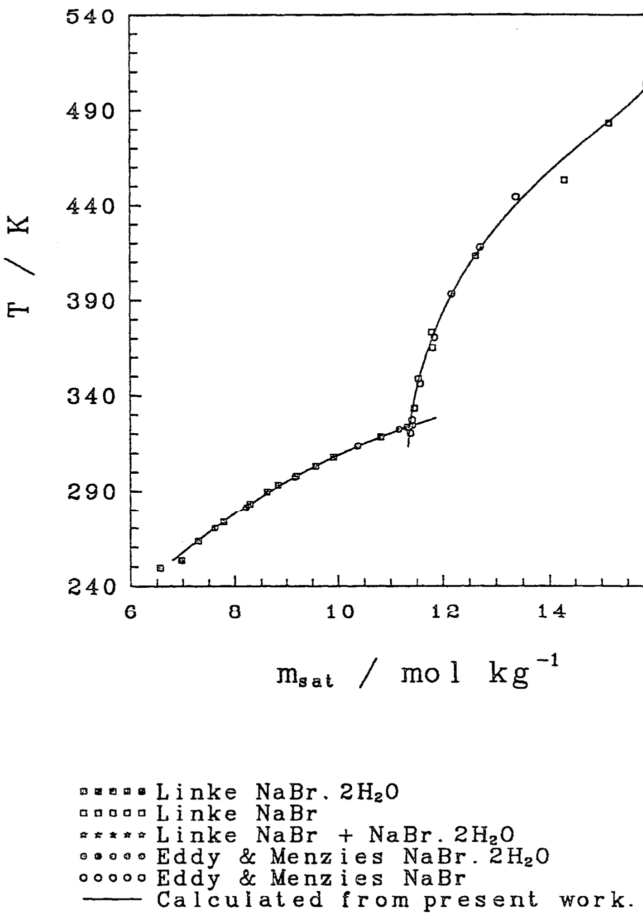

FIG. 17. Values of the solubility of NaBr(cr) and NaBr·2H_2O(cr) calculated from the equation for the solution properties combined with thermodynamic properties of the solid phases from the present work.

solubility and large temperature for NaBr(aq), the value of the solute activity coefficient becomes small, and the calculated solubilities become very susceptible to small uncertainties in the small activity coefficient. Thus the agreement for 400 to 500 K was considered to be very satisfactory. The 298.15 K Gibbs energies and enthalpies of formation for NaBr(cr) and NaBr·2H_2O(cr), given in Table 5, were calculated from the parameters given in Table 2 and the values of Cox *et al.*[17] for $\Delta_f H^\circ_m$ and $S^\circ_{2,m}$ for NaBr(aq), H_2O and the elements.

The 298.15 K, 0.1 MPa standard-state enthalpies of solution calculated from the present work are given in Table 6. Also given in this table are the recommended values from Parker,[83] as well as some of the values calculated from enthalpies of solution reported in the literature. (Values prior to the change of the century have not been tabulated.) The literature values for anhydrous NaBr range from -0.2 to -1.0 kJ·mol^{-1}. This large range of experimental value suggests the possibility of systematic error sources in the measurements; thus these results were not included in the least-squares procedure. The enthalpy of solution for the anhydrous phase obtained from the values given by Lange and Dürr[84] and by Rabinovich[85] were both in reasonable agreement with the value obtained from the global fit. The remaining values were all less exothermic than the present value. Lange and Dürr inadvertently compared their measured enthalpy of solution to a value of the partial molar enthalpy of solution given by Wüst and Lange,[87] and so missed the opportunity to comment on the significant difference between their value and the earlier measurements. The value from Samoilov[91] for the dihydrate was slightly more endothermic than the present value, however, this agreement was considered reasonable. The value recommended by Parker was calculated from values given by Thomsen,[92] and was less endothermic than the present value.

The simplest explanation for the differences of most of the experimental values amongst themselves and from the present calculated values was incomplete stoichiometry of the solid samples. In other words, the NaBr(cr) was not completely anhydrous, and the NaBr·2H_2O was not completely hydrated. The values of the two calculated enthalpies of solution indicate: 1) a not-completely-anhydrous sample of the NaBr(cr) would exhibit an observed enthalpy of solution less exothermic than the true value; and 2) a not-completely-hydrated sample of NaBr·2H_2O would exhibit an observed enthalpy of solution less endothermic than the true value. These two observations were in agreement with the differences from the present

TABLE 5. The Gibbs energy and enthalpy of formation of NaBr(cr) and $NaBr{\cdot}2H_2O(cr)$ for 298.15 K and 0.1 MPa caculated from the least-squares estimated parameters.[a]

Substance	$\Delta_f G_m^\circ$	$\Delta_f H_m^\circ$
NaBr	-348.79	-360.89
$NaBr{\cdot}2H_2O$	-828.30	-952.30

[a] Units are $kJ{\cdot}mol^{-1}$.

calculated values of the experimental values from the literature and from Parker's[83] recommended values. An estimate of the effect of incomplete stoichiometry can be made if an approximately additive effect for the waters of hydration is assumed. With this assumption, the error in the enthalpy of solution for 0.5% water content (by weight) in the NaBr(cr) sample was estimated to be aproximately 300 $J{\cdot}mol^{-1}$. This value is approximately the size of the difference between Parker's recommended value for NaBr(cr) and that calculated from the globally fitted equations for NaBr + H_2O. It is also observed that, for 298.15 K, the equilibrium vapor pressure of water over the dihydrate is approximately one third of the vapor pressure of pure water. This vapor pressure may have caused difficulty in maintaining either the anhydrous or the hydrated phase samples in their completely hydrated or completely dehydrated states.

Of course, alternative explanations for the discrepancies of the solubility calculated from Wagman *et al.*'s thermodynamic properties as well as the discrepancy of the 298.15 K $\Delta_{sol}H_m^\circ$ calculated from the fitted parameters and the experimental values were possible. One of these explanations was that the values of the 298.15 K thermodynamic properties of NaBr(aq), given in Refs. 82 and 17, were both significantly in error. This explanation seemed the more unlikely, if only because there existed at least some explanation as to how these values were obtained in Ref. 17, and because these results were obtained on an individual-ion basis. Additionally, the possibility remains that substantial errors in the isopiestic molality determinations for 298.15 K, 0.1 MPa and molalities greater than 4 $mol{\cdot}kg^{-1}$. Neither of these possibilities could be eliminated from consideration in the present work.

5. $NaBr{\cdot}2H_2O(cr) = NaBr(cr) + 2H_2O(g)$

The vapor pressure of water above $NaBr{\cdot}2H_2O(cr)$ provides another source of quantitative information regarding the Gibbs energies of formation for NaBr(cr) and $NaBr{\cdot}2H_2O(cr)$. The vapor pressure results of Dingemanns,[74] from 283.15 to 323.75 K, were also included in the least-squares procedure. Fig. 18 shows the difference between the decomposition pressures reported by Bell[93] and by Dingemans and that calculated from Eq. (33). Also shown are values given by Brönsted and Peterson,[98] Schoorl,[99] Flood,[100] and Jensen and Lannung.[99] The agreement with Dingemans' results is within twice his stated uncetainty of 0.013 kPa, for all temperatures.

Agreement with Flood's value is within his stated uncertainty of 0.007 kPa. Also shown in the figure are values of the decomposition pressure calculated from values of the Gibbs energies of formation and the molar entropies reported by Wagman *et al.*[82] and the heat capacities of water and the solid phases reported here. Values of the decomposition pressure from Watelle-Marion *et al.*[95] were not considered because their vapor-pressure curve for the saturated solution did not intersect the decomposition pressure curve near 323 K. Extrapolation of their equations for the respective vapor pressures gave 366 K as the intersection temperature, a value significantly different from the triple point reported for the solubility measurements and for Dingemans' vapor-pressure measurements.

TABLE 6. The enthalpy of solution of NaBr(cr) and $NaBr{\cdot}2H_2O(cr)$ for 298.15 K and 0.1 MPa.[a]

Substance	$\Delta_{sol}H_m^\circ$ calculated from the least-squares parameters	$\Delta_{sol}H_m^\circ$ "recommended" value of Ref. 83	$\Delta_{sol}H_m^\circ$ literature values	Ref.
NaBr	−0.86	−0.602 ± 0.063	−1.023	84
			−1.026	85
			−0.657	86
			−0.623	87
			−0.606	93
			−0.603	66
			−0.573	88
			−0.55	90
			−0.22	89
$NaBr{\cdot}2H_2O$	18.9	18.636 ± 0.21	19.1	91

[a] Units are $kJ{\cdot}mol^{-1}$.

6. Estimation of Uncertainty and Calculated Values

It is nearly impossible to reliably estimate the uncertainty in calculated values for a system such as the present, for which so many of the experimental measurements were found to be inconsistent with each other. Uncertainty in the osmotic coefficients for 298.15 K, 0.1 MPa and for molalities less than 5 mol·kg^{-1} is probably ±0.005; for molalities between 5 and 9 mol·kg^{-1} the uncertainty is approximately ±0.01 to 0.02. The probable uncertainty in activity coefficients for 298.15 K, 0.1 MPa, and for molalities less than 5 mol·kg^{-1} is ±0.01; for molalities between 5 and 9 mol·kg^{-1}, it is approximately ±0.02 to 0.03. Because the enthalpy of dilution and heat-capacity results were in good agreement, the changes in activity and osmotic coefficients with respect to temperature were fairly well characterized. Thus, the uncertainties in osmotic and activity coefficients should not be expected to increase by more than a factor of two from the values for 298.15 K, for temperatures less than 500 K. For temperatures above 500 K, the ability to integrate the osmotic and activity coefficients for molalities greater than 5 mol·kg^{-1} decreased because the heat-capacity results for this temperature range extended only to 3 mol·kg^{-1}, the concentration dependence of the integration is less well-defined with heat-capacity results than with enthalpy-of-dilution results (this is true even for 298.15 K[97]), and the activity and osmotic coefficients changed more rapidly with temperature and pressure. The uncertainties in osmotic coefficient and logarithm of the activity coefficient for 575 – 600 K might be expected to be as large as 0.02 – 0.1, dependent upon concentration and pressure.

The uncertainties in apparent molar volumes and densities were essentially those from the following investigators for the respective temperature, pressure and concentration regions: Gibson and Loeffler[35,36] for 298.15 – 358.15 K, 0.1 – 100 MPa, and 0 – 9 mol·kg^{-1}; twice the uncertainty given by Majer *et al.*[41] for 358.15 – 575 K, p_w – 50 MPa, and 0 – 3 mol·kg^{-1}; Baxter and Wallace[32] for 273.15 – 298.15, 0.1 MPa, and 0 – 9 mol·kg^{-1}. In temperature and pressure regions outside of these, a smooth transition from these uncertainties to those of Egorov *et al.*[37] was expected. As temperature decreases from 298.15 K and for pressures increasing from ambient, the

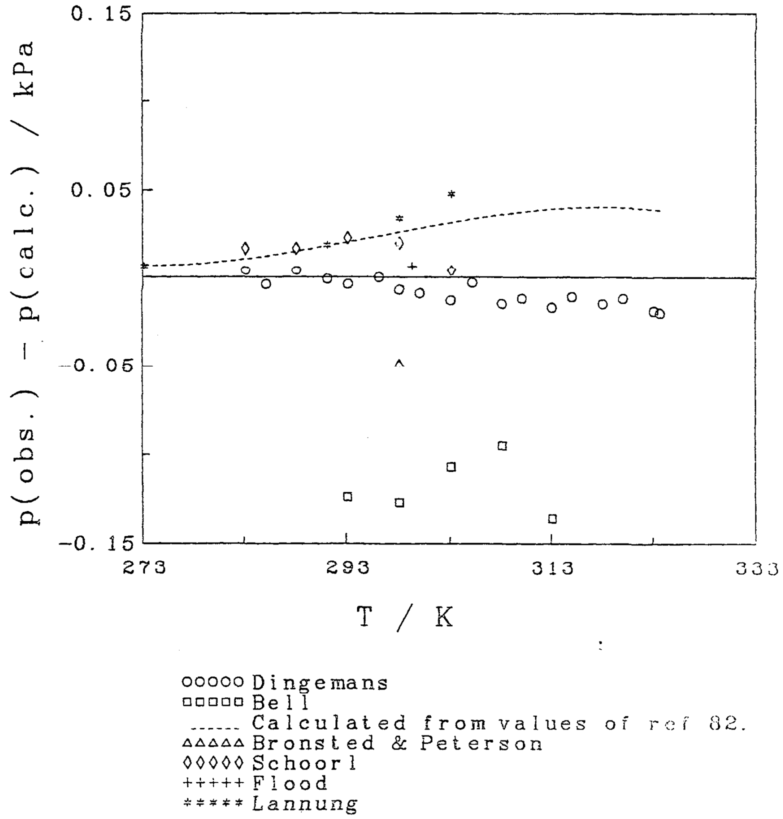

FIG. 18. The difference of the decomposition pressure for NaBr·$2H_2O$(cr) calculated from the present work and experiment. Also shown are values calculated from the values of Wagman *et al.*

uncertainty in apparent molar volumes and in the changes of Gibbs energy, enthalpy, entropy and heat capacity with respect to pressure might become large, because of the lack of thermodynamic results for this region of T and p.

Because the total number of properties which can be calculated from the present equations is so large, no attempt was made to generate tables of all properties for the present work. Tables for a very few selected properties appear at the end of this paper. These calculated properties for NaBr(aq) are: the change in standard-state molar Gibbs energy and molar enthalpy from the values for T_r and p_r, standard-state molar entropy, activity coefficient, osmotic coefficient, apparent molar volume, and density of solvent and solution.

Note added in proof: Recently, Majer *et al.* (V. Majer, L. Hui, R. Crovetto, R. H. Wood, J. Chem. Thermodynamics, **23**, 301 (1991).) have reported values of $\rho_s - \rho_w$ for NaBr(aq) from 604.4 to 725.5 K and from 0.005 to 3.0 mol·kg^{-1}. Values of $\rho_s - \rho_w$ calculated from the present equations for 604.4 K agree with their results within their experimental precision, for molalities less than 0.1 mol·kg^{-1} and for their three pressures. For molalities greater than 0.1 mol·kg^{-1} for 604.4 K, and their three pressures, the present equations provide values of V_Φ that have a r.m.s. deviation of 2.8 cm^3·mol^{-1}. For these same conditions, values of $\rho_s - \rho_w$ calculated from the present equations are an average of 1.4 percent larger than their results. This difference in $\rho_s - \rho_w$ corresponds to differences of 0.02, 0.1, 0.17 and 0.4 percent in solution density for molalities of 0.1, 0.5, 1.0 and 3.0 mol·kg^{-1}, respectively. This difference in $\rho_s - \rho_w$, for molalities greater than 0.1 mol·kg^{-1}, is about a factor of three larger than the absolute accuracy of the calibration of the instrument for lower temperatures for NaCl(aq) and so the present level of agreement can be considered an acceptable verification of the present equation.

7. Acknowledgment

Dr. J. Rard brought Ref. 60 to my attention; this reference prompted significant changes in this work. The helpful comments and suggestions of Dr. D. G. Garvin, Prof. R. H. Wood, Dr. V. Majer, Dr. P. A. G. O'Hare and Dr. R. N. Goldberg were greatly appreciated.

8. References

[1] P. G. Hill, J. Phys. Chem. Ref. Data **19** 1233 (1990)

[2] L. B. Pankratz, Thermodynamic Properties of Halides, USBM Bulletin 674, (1984).

[3] K. K. Kelley, High-Temperature Heat-Content, Heat-Capacity, and Entropy Data for the Elements and Inorganic Compounds, USBM Bulletin 584 (1960).

[4] A. Magnus, Phys. Zeitschrift. **14**, 5 (1913).

[5] T. E. Gardner, A. R. Taylor, High-Temperature Heat Contents and Entropies of Sodium Bromide and Sodium Iodide, U.S. Bureau of Mines, RI 7040 (1967).

[6] T. E. Gardner, A. R. Taylor, Thermodynamic Properties of Sodium Bromide and Sodium Iodide at Low Temperatures, USBM RI6435 (1964).

[7] W. T. Berg, J. A. Morrison, Proc. Roy. Soc. (London) **A242**, 467 (1957).

[8] J. A. Morrison, D. Patterson, Trans. Faraday Soc. **52**, 764 (1956).

[9] D. C. Ginnings, G. T. Furukawa, J. Amer. Chem. Soc. **75**, 522 (1953).

[10] J. A. Birch, J. G. Collins, G. K. White, Aust. J. Phys. **32**, 463 (1979).

[11] G. P. Baxter, C. C. Wallace, J. Amer. Chem. Soc. **38**, 259 (1916).

[12] K. S. Pitzer, J. Phys. Chem. **77**, 268 (1973).

[13] As an example see: K. S. Pitzer, J. C. Peiper, R. H. Busey, J. Phys. Chem. Ref. Data **13**, 1 (1984) and references cited therein.

[14] D. G. Archer, P. Wang, J. Phys. Chem. Ref. Data **19**, 371 (1990)

[15] D. J. Bradley, K. S. Pitzer, J. Phys. Chem. **83**, 1599 (1979).

[16] P. S. Z. Rogers, K. S. Pitzer, J. Phys. Chem. Ref. Data **11**, 15 (1982).

[17] J. D. Cox, D. D. Wagman, V. A. Medvedev, CODATA Key Values for Thermodynamics, (Hemisphere, Washington) (1989).

[18] See for example: J. D. Frantz, W. L. Marshall, Am. J. Sci. **284**, 651 (1984) and references described therein.

[19] D. G. Archer, Ph.D. Dissertation, Univ. of Delaware (1984).

[20] H. F. Holmes, R. H. Busey, J. M. Simonson, R. E. Mesmer, D. G. Archer, R. H. Wood, J. Chem. Thermodynamics **19**, 863 (1987).

[21] A. F. Scott, W. R. Frazier, J. Phys. Chem. **31**, 459 (1927).

[22] W. Geffcken, D. Price, Z. Physik. Chem. **B26**, 81 (1934).

[23] W. Geffcken, A. Kruis, L. Solana, Z. Physik. Chem. **B35**, 317 (1937).

[24] T. Batuecas, M. Concepcion Varela, Rev. Real Acad. Cienc. Exactas Fis. Natur. Madrid, **61**, 189 (1967).

[25] J. E. Desnoyers, M. Arel, G. Perron, C. Jolicoeur, J. Phys. Chem. **73**, 3346 (1969).

[26] F. Vaslow, J. Phys. Chem. **73**, 3745, (1969).

[27] J. L. Fortier, P. A. LeDuc, J. E. Desnoyers, J. Solution Chem. **3**, 323 (1974).

[28] F. T. Gucker, D. Stubley, D. J. Hill, J. Chem. Thermodynamics **7**, 865, (1975).

[29] F. J. Millero, G. K. Ward, P. V. Chetirkin, J. Acoust. Soc. Am. **61**, 1492 (1977).

[30] M. Kh. Karapet'yants, V. A. Vasilev, B. V. Mikhailin, V. N. Strakhov, Russ. J. Phys. Chem. **53**, 111 (1979).

[31] W. Grzybowski, G. Atkinson, J. Chem. Eng. Data **31**, 309 (1986).

[32] G. P. Baxter, C. C. Wallace, J. Amer. Chem. Soc. **38**, 70 (1916).

[33] A. F. Scott, E. J. Durham, J. Phys. Chem. **34**, 1424 (1930).

[34] Z. Shibata, P. Hθleman, Z. Physik. Chem. **B13**, 347 (1931).

[35] R. E. Gibson, O. H. Loeffler, J. Amer. Chem. Soc. **63**, 443 (1941).

[36] R. E. Gibson, O. H. Loeffler, Annal. N.Y. Acad. Sci. **51**, 727 (1949).

[37] V. A. Egorov, V. I. Zarembo, M. K. Federov, Specific Volume and Partial Characteristics of the NaBr-H_2O and NaI-H_2O Systems at Temperatures of 298-623 K and Pressures to 150 MPa, VINITI (1976).

[38] I. N. Maksimova, Ch. S. Pak, N. N. Pravdin, V. E. Razvaev, S. V. Sergeev, Yu. N. Ustinov, Physicochemical Properties of Electrolyte Solutions over a Wide Range of Temperatures and Concentrations, VINITI (1984).

[39] T. Isono, J. Chem. Eng. Data **29**, 45 (1984).

[40] J. A. Gates, R. H. Wood, J. Chem. Eng. Data **30**, 44 (1985).

[41] V. Majer, A. Inglese, R. H. Wood, J. Chem. Thermodynamics **21**, 397 (1989).

[42] H. E. Boeke, Z. Krist. **45**, 360 (1908).

[43] Sodev Inc., P.O. Box 1060, Sherbrooke, Canada J1H 5LB.

[44] D. G. Archer, V. Majer, A. Inglese, R. H. Wood, J. Colloid Interf. Sci. **124**, 591 (1988).

[45] V. Majer, J. A. Gates, A. Inglese, R. H. Wood, J. Chem. Thermodynamics, **20**, 949 (1989).

[46] F. J. Millero in Activity Coefficients in Electrolyte Solutions, R. N. Pytkowicz, ed. (C.R.C. Press, Boca Raton, FL 1979).

[47] H. S. Harned, B. B. Owen, ACS Monograph Series, No. 137 (Reinhold, New York, 1958).

[48] J. G. Mathieson, B. E. Conway, J. Solution Chem. **3**, 455 (1974).

[49] H. S. Harned, S. M. Douglas, J. Amer. Chem. Soc. **48**, 3095 (1926).

[50] H. S. Harned, J. Amer. Chem. Soc. **51**, 416 (1929).

[51] H. S. Harned, C. C. Crawford, J. Amer. Chem. Soc. **59**, 1903 (1937).

[52] V. I. Lebed, V. V. Aleksandrov, Rus. J. Phys. Chem. (English) **38**, 1414 (1964).

[53] G. Scatchard, S. S. Prentiss, J. Amer. Chem. Soc. **55**, 4355, (1933).

[54] G. Damköhler, J. Weinzierl, Z. Physik. Chem. A167, **71** (1933).

[55] R. A. Robinson, J. Amer. Chem. Soc. **57**, 1161 (1935).

[56] R. H. Stokes, R. A. Robinson, Ind. Eng. Chem. **41**, 2013 (1949).

[57] J. Penciner, Y. Marcus, J. Chem. Eng. Data **10**, 105 (1965).

[58] L. L. Makarov, Yu. G. Vlasov, V. A. Azarko, Russian J. Phys. Chem. (English) **40**, 609, (1966).

[59] A. K. Covington, T. H. Lilley, R. A. Robinson, J. Phys. Chem. **72**, 2759 (1968).

[60] A.N. Kirgintsev, A. V. Luk'yanov, Russ. J. Phys. Chem. (Eng.) **38**, 867 (1964).

[61] J. N. Pearce , M. D. Taylor, R. M. Bartlett, J. Amer. Chem. Soc. **50**, 2951 (1928).

[62] D. S. Carr, B. L. Harris, Ind. Eng. Chem. **41**, 2014 (1949).

[63] G. Jakli, W. A. Van Hook, J. Chem. Eng. Data **17**, 348 (1972).

[64] V. P. Mashovets, V. I. Zarembo, M. K. , Zhurnal Prikladnoi Khimii, **46**, 650 (1973).

[65] H. Hammerschmid, A. L. Robinson, J. Amer. Chem. Soc. **54**, 3120 (1932).

[66] W. E. Wallace, J. Amer. Chem. Soc. **71**, 2485 (1949).

[67] F. Vaslow, J. Phys. Chem. **75**, 3317 (1971).

[68] R. H. Wood, R. A. Rooney, J. N. Braddock, J. Phys. Chem. **73**, 1673 (1969).

[69] W. H. Leung, F. J. Millero, J. Chem. Thermodynamics **7**, 1067 (1975).

[70] J. E. Mayrath, R. H. Wood, J. Chem. Thermodynamics **14**, 563 (1982).

[71] M. Randall, F. D. Rossini, J. Amer. Chem. Soc. **51**, 323 (1929).

[72] J. E. Tanner, F. W. Lamb, J. Solution Chem. **7**, 303 (1978).

[73] D. E. White, J. A. Gates, R. H. Wood, J. Chem. Thermodynamics **19**, 493 (1987).

[74] P. Dingemans, Rec. Trav. Chim. **57**, 703 (1935).

[75] Q. D. Craft, W. A. Van Hook, J. Solution Chem. **4**, 923, (1975).

[76] R. H. Wood, personal communication.

[77] W. J. Hamer, Y.-C. Wu, J. Phys. Chem. Ref. Data **1**, 1047 (1972).

[78] E. C. W. Clarke, D. N. Glew, J. Phys. Chem. Ref. Data **14**, 489, (1985).

[79] D. Garvin, V. B. Parker, H. J. White, CODATA Thermodynamic Tables (Hemisphere, Washington, D.C. 1987).

[80] W. F. Linke, Solubilities of Inorganic and Metal-Organic Compounds, Vol. 2 (American Chemical Society, Washington, D.C. 1965)

[81] R. D. Eddy, A. W. C. Menzies, J. Phys. Chem. **44**, 207 (1940).

[82] D. D. Wagman, W. H. Evans, V. B. Parker, R. H. Schumm, I. Halow, S. M. Bailey, K. L. Churney, R. L. Nuttall, J. Phys. Chem. Ref. Data **11**, Suppl. 2 (1982).

[83] V. B. Parker, Thermal Properties of Aqueous Uni-univalent Electrolytes, (U.S. Department of Commerce, NSRDS-NBS 2, Washington, 1965).

[84] E. Lange, F. Dürr, Z. Elektrochem. **32**, 85, (1926).

[85] I. B. Rabinovich, V. G. Tsvetkov, Russ. J. Phys. Chem. (English) **45**, 1518 (1971).

[86] R. D. Joly, G. Perachon, Thermochim. Acta **21**, 333 (1977).

[87] J. Wüst, E. Lange, Z. Physik. Chem. **116**, 161 (1925).

[88] Q. D. Craft, W. A. Van Hook, J. Solution Chem. **4**, 901 (1975).

[89] C. M. Slansky, J. Amer. Chem. Soc. **62**, 2430 (1940).

[90] R. Fuchs, C. P. Hagan, J. Phys. Chem. **77**, 1797 (1973).

[91] O. Ya. Samoilov, Izv. Akad. Nauk S.S.S.R., Otdel, Khim. Nauk, 398 (1952).

[92] J. Thomsen, Thermochemische Untersuchen (J. Barth Verlag, Leipzig, 1882) .

[93] F. A. Askew, E. Bullock, H. T. Smith, R. K. Tinkler, O. Gatty, J. H. Wolfenden, J. Chem. Soc. 1368 (1934).

[94] J. Bell, J. Chem. Soc. 459 (1937).

[95] G. Watelle-Marion, A. Thrierr-Sorel, M. Lallemant, Compt. Rend. **259**, 4679 (1964).

[96] D. G. Archer, R. H. Wood, J. Solution Chem. **14**, 757 (1985).

[97] D. G. Archer, J. Phys. Chem. **93**, 5272 (1989).

[98] J. N. Brönsted, A. Peterson, Kgl. Danske Videnskol. Selskab., Math. fys. Medd., **3**, 7 (1917) as reported in Ref. 92.

[99] N. Schoorl, Kommentar zur Niederl. Pharmacopee **1** 30 u. 31 (1927), as reported in Ref. 92.

[100] E. A. Flood, Can. J. Chem., **31**, 993 (1954).

[101] A. T. Jensen, A. Lannung, Kgl. Danske Videnskol. Selskab., Math. fys. Medd., **20**, 3 (1943)

[102] W. T. Richards, Rev. Mod. Phys. **11**, 36 (1939).

Appendix

Table A-1. The calculated standard-state molar Gibbs energy of NaBr(aq), relative to 298.15 K and 0.1 MPa, $G^{\circ}_{\mathrm{m},2} - G^{\circ}_{\mathrm{m},2,T_r,p_r}$. Units are kJ·mol^{-1}

T/K	p^a	0.1 MPa/p_w	10 MPa	25 MPa	50 MPa	75 MPa	100 MPa
273.15	0.1	3.655	3.866	4.194	4.762	5.353	5.965
278.15	0.1	2.897	3.117	3.457	4.042	4.649	5.273
283.15	0.1	2.156	2.382	2.732	3.332	3.951	4.586
288.15	0.1	1.427	1.659	2.017	2.628	3.258	3.903
293.15	0.1	0.709	0.945	1.310	1.931	2.569	3.222
298.15	0.1	0.000	0.240	0.610	1.239	1.885	2.545
303.15	0.1	−0.701	−0.458	−0.084	0.552	1.204	1.869
308.15	0.1	−1.396	−1.150	−0.773	−0.131	0.526	1.196
313.15	0.1	−2.084	−1.837	−1.456	−0.810	−0.149	0.525
318.15	0.1	−2.767	−2.518	−2.136	−1.485	−0.821	−0.144
323.15	0.1	−3.444	−3.195	−2.811	−2.158	−1.491	−0.812
328.15	0.1	−4.117	−3.866	−3.481	−2.827	−2.158	−1.477
333.15	0.1	−4.785	−4.534	−4.148	−3.493	−2.823	−2.141
338.15	0.1	−5.448	−5.197	−4.812	−4.156	−3.486	−2.803
343.15	0.1	−6.106	−5.856	−5.471	−4.816	−4.146	−3.463
348.15	0.1	−6.760	−6.511	−6.127	−5.473	−4.803	−4.121
353.15	0.1	−7.410	−7.161	−6.778	−6.126	−5.458	−4.777
358.15	0.1	−8.054	−7.807	−7.426	−6.776	−6.111	−5.431
363.15	0.1	−8.694	−8.449	−8.070	−7.423	−6.760	−6.082
368.15	0.1	−9.329	−9.086	−8.710	−8.067	−7.407	−6.732
373.15	0.1	−9.960	−9.718	−9.346	−8.707	−8.051	−7.379
383.15	0.1	−11.203	−10.969	−10.604	−9.976	−9.329	−8.665
393.15	0.2	−12.425	−12.199	−11.844	−11.230	−10.594	−9.939
398.15	0.2	−13.027	−12.806	−12.456	−11.851	−11.221	−10.572
403.15	0.3	−13.623	−13.407	−13.064	−12.467	−11.845	−11.202
413.15	0.4	−14.796	−14.592	−14.263	−13.686	−13.080	−12.451
423.15	0.5	−15.941	−15.751	−15.439	−14.885	−14.299	−13.687
433.15	0.6	−17.056	−16.883	−16.590	−16.064	−15.500	−14.907
443.15	0.8	−18.137	−17.984	−17.714	−17.219	−16.682	−16.110
448.15	0.9	−18.665	−18.522	−18.265	−17.788	−17.265	−16.705
453.15	1.0	−19.183	−19.051	−18.808	−18.351	−17.842	−17.295
463.15	1.3	−20.189	−20.082	−19.870	−19.455	−18.981	−18.462
473.15	1.6	−21.152	−21.072	−20.897	−20.531	−20.096	−19.608
498.15	2.5	−23.334	−23.336	−23.285	−23.078	−22.765	−22.375
523.15	4.0	−25.116	−25.211	−25.354	−25.382	−25.238	−24.979
548.15	5.9	−26.350	−26.524	−26.991	−27.376	−27.472	−27.389
573.15	8.6	−26.786	−26.925	−28.008	−28.966	−29.407	−29.562
598.15	12.0	−25.943		−28.059	−30.019	−30.963	−31.436

[a] Column gives the pressure for values of $G^{\circ}_{\mathrm{m},2} - G^{\circ}_{\mathrm{m},2,T_r,p_r}$ in the 0.1 MPa/p_w column.

Table A-2. The calculated standard-state molar enthalpy of NaBr(aq), relative to 298.15 K and 0.1 MPa, $H^{\circ}_{\mathrm{m},2} - H^{\circ}_{\mathrm{m},2,T_r,p_r}$. Units are kJ·mol^{-1}

T/K	p^a	0.1 MPa/p_w	10 MPa	25 MPa	50 MPa	75 MPa	100 MPa
273.15	0.1	3.517	3.214	2.820	2.319	1.983	1.783
278.15	0.1	2.525	2.325	2.071	1.769	1.596	1.531
283.15	0.1	1.722	1.601	1.456	1.309	1.265	1.307
288.15	0.1	1.055	0.998	0.941	0.920	0.981	1.110
293.15	0.1	0.490	0.485	0.500	0.584	0.733	0.936
298.15	0.1	0.000	0.039	0.116	0.289	0.512	0.779
303.15	0.1	−0.434	−0.357	−0.227	0.024	0.313	0.634
308.15	0.1	−0.828	−0.717	−0.539	−0.220	0.128	0.499
313.15	0.1	−1.190	−1.049	−0.829	−0.447	−0.047	0.370
318.15	0.1	−1.531	−1.362	−1.103	−0.664	−0.215	0.243
323.15	0.1	−1.858	−1.663	−1.367	−0.875	−0.380	0.117
328.15	0.1	−2.174	−1.955	−1.625	−1.082	−0.544	−0.011
333.15	0.1	−2.486	−2.243	−1.881	−1.289	−0.710	−0.141
338.15	0.1	−2.797	−2.531	−2.137	−1.498	−0.879	−0.277
343.15	0.1	−3.109	−2.821	−2.395	−1.711	−1.054	−0.418
348.15	0.1	−3.427	−3.116	−2.660	−1.931	−1.234	−0.566
353.15	0.1	−3.751	−3.418	−2.931	−2.157	−1.423	−0.722

Table A-2. The calculated standard-state molar enthalpy of NaBr(aq), relative to 298.15 K and 0.1 MPa, $H^{\circ}_{m,2} - H^{\circ}_{m,2,T_r,p_r}$. Units are kJ·mol^{-1} – Continued

T/K	p^a	0.1 MPa/p_w	10 MPa	25 MPa	50 MPa	75 MPa	100 MPa
358.15	0.1	−4.085	−3.729	−3.211	−2.392	−1.620	−0.887
363.15	0.1	−4.430	−4.051	−3.501	−2.637	−1.827	−1.062
368.15	0.1	−4.788	−4.385	−3.803	−2.892	−2.044	−1.247
373.15	0.1	−5.160	−4.734	−4.118	−3.160	−2.272	−1.442
383.15	0.1	−5.954	−5.478	−4.791	−3.734	−2.765	−1.868
393.15	0.2	−6.826	−6.295	−5.531	−4.367	−3.311	−2.343
398.15	0.2	−7.295	−6.735	−5.929	−4.707	−3.605	−2.600
403.15	0.3	−7.789	−7.198	−6.348	−5.065	−3.915	−2.870
413.15	0.4	−8.857	−8.199	−7.251	−5.835	−4.582	−3.455
423.15	0.5	−10.048	−9.314	−8.252	−6.687	−5.318	−4.100
433.15	0.6	−11.379	−10.558	−9.364	−7.627	−6.128	−4.809
443.15	0.8	−12.873	−11.953	−10.603	−8.666	−7.019	−5.588
448.15	0.9	−13.689	−12.714	−11.275	−9.225	−7.497	−6.004
453.15	1.0	−14.556	−13.522	−11.985	−9.814	−7.998	−6.440
463.15	1.3	−16.460	−15.295	−13.532	−11.086	−9.074	−7.371
473.15	1.6	−18.625	−17.307	−15.269	−12.495	−10.256	−8.388
498.15	2.5	−25.526	−23.716	−20.662	−16.744	−13.752	−11.357
523.15	4.0	−35.592	−33.106	−28.170	−22.348	−18.209	−15.058
523.15	4.0	−35.592	−33.106	−28.170	−22.348	−18.209	−15.058
548.15	5.9	−51.202	−47.972	−39.094	−29.893	−23.962	−19.717
573.15	8.6	−77.880	−75.168	−56.055	−40.302	−31.513	−25.713
598.15	12.0	-132.295		−85.088	−54.896	−41.679	−33.932

[a] Column gives the pressure for values of $H^{\circ}_{m,2} - H^{\circ}_{m,2,T_r,p_r}$ in the 0.1 MPa / p_w column

Table A-3. The calculated standard-state entropy, $S^{\circ}_{2,m}$, of NaBr(aq). Units are kJ·K^{-1}·mol^{-1}

T/K	p^a	0.1 MPa/p_w	10 MPa	25 MPa	50 MPa	75 MPa	100 MPa
273.15	0.1	0.153	0.152	0.149	0.145	0.142	0.139
278.15	0.1	0.150	0.148	0.146	0.143	0.140	0.138
283.15	0.1	0.147	0.146	0.144	0.141	0.139	0.137
288.15	0.1	0.145	0.144	0.142	0.140	0.138	0.136
293.15	0.1	0.143	0.142	0.141	0.139	0.137	0.136
298.15	0.1	0.141	0.140	0.139	0.138	0.136	0.135
303.15	0.1	0.140	0.139	0.138	0.137	0.136	0.135
308.15	0.1	0.138	0.138	0.137	0.136	0.135	0.134
313.15	0.1	0.137	0.137	0.136	0.135	0.135	0.134
318.15	0.1	0.136	0.136	0.135	0.135	0.134	0.133
323.15	0.1	0.135	0.135	0.135	0.134	0.134	0.133
328.15	0.1	0.134	0.134	0.134	0.133	0.133	0.133
333.15	0.1	0.133	0.133	0.133	0.133	0.133	0.132
338.15	0.1	0.132	0.132	0.132	0.132	0.132	0.132
343.15	0.1	0.131	0.131	0.131	0.132	0.132	0.131
348.15	0.1	0.130	0.131	0.131	0.131	0.131	0.131
353.15	0.1	0.129	0.130	0.130	0.130	0.130	0.131
358.15	0.1	0.128	0.129	0.129	0.130	0.130	0.130
363.15	0.1	0.128	0.128	0.128	0.129	0.129	0.130
368.15	0.1	0.127	0.127	0.128	0.128	0.129	0.129
373.15	0.1	0.126	0.126	0.127	0.128	0.128	0.129
383.15	0.1	0.123	0.124	0.125	0.126	0.127	0.127
393.15	0.2	0.121	0.122	0.123	0.124	0.125	0.126
398.15	0.2	0.120	0.121	0.122	0.124	0.125	0.126
403.15	0.3	0.119	0.120	0.121	0.123	0.124	0.125
413.15	0.4	0.116	0.117	0.119	0.121	0.122	0.124
423.15	0.5	0.113	0.115	0.116	0.119	0.121	0.122
433.15	0.6	0.110	0.112	0.114	0.117	0.119	0.120
443.15	0.8	0.107	0.108	0.111	0.114	0.117	0.119
448.15	0.9	0.105	0.107	0.109	0.113	0.116	0.118
453.15	1.0	0.103	0.105	0.108	0.112	0.114	0.117
463.15	1.3	0.099	0.101	0.104	0.109	0.112	0.115
473.15	1.6	0.094	0.097	0.101	0.106	0.110	0.113
498.15	2.5	0.080	0.084	0.090	0.097	0.102	0.107
523.15	4.0	0.060	0.065	0.075	0.086	0.094	0.099

Table A-3. The calculated standard-state entropy, $S^\circ_{2,m}$, of NaBr(aq). Units are kJ·K-1·mol^{-1} — Continued

T/K	p^a	0.1 MPa/p_w	10 MPa	25 MPa	50 MPa	75 MPa	100 MPa
548.15	5.9	0.031	0.038	0.055	0.072	0.083	0.091
573.15	8.6	−0.016	−0.011	0.024	0.054	0.070	0.080
598.15	12.0	−0.108		−0.025	0.029	0.052	0.066

[a] Column gives the pressure for values of the standard-state entropy in the 0.1 MPa / p_w column.

Table A-4. The calculated activity coefficient, $\gamma_\pm$, of NaBr(aq)

		m / mol·kg^{-1}							
T/K	p/ MPa	0.1	0.25	0.5	1.0	2.0	4.0	6.0	8.0
273.15	0.1	0.788	0.733	0.696	0.670	0.685	0.837	1.118	1.546
278.15	0.1	0.789	0.736	0.701	0.679	0.701	0.867	1.162	1.597
283.15	0.1	0.789	0.737	0.704	0.686	0.714	0.892	1.199	1.641
288.15	0.1	0.789	0.738	0.707	0.692	0.725	0.913	1.230	1.677
293.15	0.1	0.789	0.739	0.709	0.696	0.733	0.931	1.255	1.706
298.15	0.1	0.788	0.738	0.709	0.699	0.740	0.945	1.276	1.728
303.15	0.1	0.787	0.738	0.710	0.701	0.746	0.956	1.292	1.743
308.15	0.1	0.786	0.737	0.709	0.702	0.750	0.965	1.303	1.753
313.15	0.1	0.784	0.736	0.709	0.703	0.752	0.971	1.311	1.757
318.15	0.1	0.783	0.734	0.708	0.702	0.754	0.975	1.315	1.756
323.15	0.1	0.781	0.732	0.706	0.702	0.754	0.977	1.316	1.751
328.15	0.1	0.779	0.730	0.704	0.700	0.754	0.978	1.315	1.742
333.15	0.1	0.777	0.728	0.702	0.698	0.752	0.976	1.310	1.729
338.15	0.1	0.775	0.725	0.699	0.696	0.750	0.973	1.303	1.713
343.15	0.1	0.773	0.723	0.696	0.693	0.748	0.969	1.294	1.693
348.15	0.1	0.770	0.720	0.693	0.690	0.744	0.963	1.283	1.671
353.15	0.1	0.768	0.717	0.690	0.687	0.740	0.956	1.269	1.647
358.15	0.1	0.765	0.714	0.687	0.683	0.736	0.949	1.255	1.621
363.15	0.1	0.763	0.711	0.683	0.678	0.730	0.940	1.239	1.592
368.15	0.1	0.760	0.707	0.679	0.674	0.725	0.930	1.221	1.562
373.15	0.1	0.757	0.704	0.675	0.669	0.719	0.919	1.202	1.531
383.15	0.1	0.751	0.696	0.666	0.659	0.705	0.896	1.161	1.465
393.15	0.2	0.745	0.688	0.657	0.648	0.690	0.869	1.117	1.396
398.15	0.2	0.741	0.684	0.652	0.642	0.682	0.856	1.094	1.360
403.15	0.3	0.738	0.680	0.647	0.636	0.674	0.841	1.071	1.324
413.15	0.4	0.731	0.671	0.636	0.623	0.657	0.811	1.022	1.251
423.15	0.5	0.723	0.661	0.625	0.609	0.638	0.779	0.972	1.178
433.15	0.6	0.715	0.651	0.613	0.595	0.619	0.747	0.920	1.104
443.15	0.8	0.707	0.641	0.601	0.580	0.598	0.713	0.869	1.032
448.15	0.9	0.703	0.635	0.595	0.572	0.588	0.696	0.843	0.996
453.15	1.0	0.698	0.630	0.588	0.564	0.577	0.678	0.817	0.960
463.15	1.3	0.689	0.618	0.574	0.548	0.555	0.643	0.765	0.890
473.15	1.6	0.680	0.606	0.560	0.530	0.533	0.607	0.713	0.821
498.15	2.5	0.653	0.573	0.522	0.485	0.474	0.517	0.587	0.659
523.15	4.0	0.621	0.535	0.479	0.434	0.411	0.426	0.466	0.510
548.15	5.9	0.584	0.491	0.429	0.378	0.344	0.336	0.353	0.376
573.15	8.6	0.537	0.437	0.370	0.315	0.273	0.249	0.249	0.260
598.15	12.0	0.474	0.367	0.299	0.242	0.197	0.166	0.158	0.162
273.15	10.0	0.790	0.736	0.699	0.675	0.692	0.847	1.128	1.549
278.15	10.0	0.790	0.738	0.704	0.684	0.707	0.876	1.172	1.602
283.15	10.0	0.791	0.740	0.707	0.691	0.720	0.901	1.208	1.647
288.15	10.0	0.790	0.740	0.710	0.696	0.730	0.922	1.239	1.684
293.15	10.0	0.790	0.741	0.711	0.700	0.739	0.939	1.265	1.713
298.15	10.0	0.789	0.740	0.712	0.703	0.745	0.953	1.285	1.736
303.15	10.0	0.788	0.740	0.712	0.705	0.750	0.964	1.301	1.752
308.15	10.0	0.787	0.739	0.712	0.706	0.754	0.972	1.313	1.763
313.15	10.0	0.786	0.738	0.711	0.706	0.757	0.978	1.320	1.768
318.15	10.0	0.784	0.736	0.710	0.706	0.758	0.982	1.325	1.768
323.15	10.0	0.782	0.734	0.708	0.705	0.759	0.984	1.326	1.763
328.15	10.0	0.780	0.732	0.707	0.703	0.758	0.985	1.324	1.754
333.15	10.0	0.778	0.730	0.704	0.702	0.757	0.983	1.320	1.742
338.15	10.0	0.776	0.727	0.702	0.699	0.755	0.980	1.313	1.726
343.15	10.0	0.774	0.725	0.699	0.697	0.752	0.976	1.304	1.707

Table A-4. The calculated activity coefficient, $\gamma_{\pm}$, of NaBr(aq) – Continued

		m / mol·kg^{-1}							
T/K	p/ MPa	0.1	0.25	0.5	1.0	2.0	4.0	6.0	8.0
348.15	10.0	0.772	0.722	0.696	0.693	0.749	0.970	1.293	1.686
353.15	10.0	0.769	0.719	0.693	0.690	0.745	0.964	1.280	1.662
358.15	10.0	0.767	0.716	0.689	0.686	0.740	0.956	1.266	1.636
363.15	10.0	0.764	0.713	0.686	0.682	0.735	0.947	1.250	1.609
368.15	10.0	0.762	0.710	0.682	0.678	0.730	0.938	1.233	1.579
373.15	10.0	0.759	0.706	0.678	0.673	0.724	0.927	1.214	1.548
383.15	10.0	0.753	0.699	0.669	0.663	0.710	0.904	1.174	1.483
393.15	10.0	0.747	0.691	0.660	0.652	0.696	0.878	1.130	1.415
398.15	10.0	0.743	0.687	0.655	0.646	0.688	0.864	1.108	1.379
403.15	10.0	0.740	0.682	0.650	0.640	0.680	0.850	1.084	1.344
413.15	10.0	0.733	0.674	0.640	0.627	0.663	0.820	1.036	1.272
423.15	10.0	0.726	0.664	0.629	0.614	0.644	0.789	0.986	1.199
433.15	10.0	0.718	0.655	0.617	0.600	0.625	0.757	0.936	1.126
443.15	10.0	0.710	0.645	0.605	0.585	0.605	0.723	0.884	1.054
448.15	10.0	0.706	0.639	0.599	0.577	0.595	0.706	0.859	1.018
453.15	10.0	0.702	0.634	0.593	0.570	0.585	0.689	0.833	0.983
463.15	10.0	0.693	0.623	0.579	0.553	0.563	0.654	0.781	0.913
473.15	10.0	0.683	0.611	0.566	0.537	0.541	0.619	0.730	0.845
498.15	10.0	0.657	0.579	0.528	0.492	0.482	0.529	0.603	0.681
523.15	10.0	0.626	0.541	0.485	0.442	0.419	0.438	0.481	0.530
548.15	10.0	0.589	0.497	0.435	0.385	0.351	0.346	0.365	0.391
573.15	10.0	0.539	0.440	0.374	0.318	0.277	0.253	0.254	0.266
273.15	25.0	0.792	0.739	0.704	0.682	0.702	0.862	1.144	1.554
278.15	25.0	0.793	0.741	0.708	0.690	0.717	0.890	1.186	1.609
283.15	25.0	0.793	0.743	0.712	0.697	0.729	0.914	1.222	1.655
288.15	25.0	0.792	0.743	0.714	0.701	0.738	0.934	1.253	1.693
293.15	25.0	0.792	0.744	0.715	0.705	0.746	0.950	1.278	1.724
298.15	25.0	0.791	0.743	0.716	0.708	0.753	0.964	1.298	1.748
303.15	25.0	0.790	0.743	0.716	0.710	0.757	0.974	1.314	1.765
308.15	25.0	0.789	0.742	0.716	0.711	0.761	0.983	1.326	1.777
313.15	25.0	0.788	0.740	0.715	0.711	0.763	0.989	1.334	1.783
318.15	25.0	0.786	0.739	0.714	0.710	0.765	0.992	1.339	1.783
323.15	25.0	0.784	0.737	0.712	0.710	0.765	0.994	1.340	1.780
328.15	25.0	0.782	0.735	0.710	0.708	0.765	0.995	1.338	1.772
333.15	25.0	0.781	0.733	0.708	0.706	0.763	0.993	1.334	1.760
338.15	25.0	0.778	0.730	0.706	0.704	0.761	0.990	1.328	1.746
343.15	25.0	0.776	0.728	0.703	0.701	0.759	0.986	1.319	1.728
348.15	25.0	0.774	0.725	0.700	0.698	0.755	0.981	1.308	1.707
353.15	25.0	0.772	0.722	0.697	0.695	0.751	0.974	1.296	1.684
358.15	25.0	0.769	0.719	0.693	0.691	0.747	0.967	1.282	1.659
363.15	25.0	0.767	0.716	0.690	0.687	0.742	0.958	1.266	1.632
368.15	25.0	0.764	0.713	0.686	0.683	0.736	0.949	1.249	1.603
373.15	25.0	0.761	0.709	0.682	0.678	0.731	0.938	1.231	1.573
383.15	25.0	0.756	0.702	0.674	0.668	0.718	0.916	1.192	1.509
393.15	25.0	0.750	0.695	0.665	0.658	0.703	0.890	1.149	1.442
398.15	25.0	0.746	0.691	0.660	0.652	0.696	0.877	1.127	1.408
403.15	25.0	0.743	0.687	0.655	0.646	0.688	0.863	1.104	1.373
413.15	25.0	0.737	0.678	0.645	0.634	0.671	0.834	1.057	1.302
423.15	25.0	0.730	0.669	0.635	0.621	0.654	0.804	1.008	1.231
433.15	25.0	0.722	0.660	0.624	0.607	0.635	0.772	0.959	1.159
443.15	25.0	0.715	0.650	0.612	0.593	0.616	0.740	0.909	1.088
448.15	25.0	0.711	0.645	0.606	0.586	0.606	0.723	0.883	1.053
453.15	25.0	0.706	0.640	0.600	0.578	0.596	0.706	0.858	1.019
463.15	25.0	0.698	0.629	0.587	0.563	0.575	0.673	0.808	0.950
473.15	25.0	0.689	0.618	0.574	0.547	0.554	0.638	0.758	0.883
498.15	25.0	0.665	0.588	0.539	0.504	0.498	0.552	0.635	0.723
523.15	25.0	0.637	0.554	0.499	0.458	0.439	0.464	0.516	0.576
548.15	25.0	0.604	0.515	0.455	0.407	0.376	0.377	0.405	0.442
573.15	25.0	0.564	0.467	0.403	0.349	0.310	0.292	0.301	0.323
598.15	25.0	0.512	0.408	0.340	0.284	0.239	0.209	0.206	0.220
273.15	50.0	0.796	0.745	0.712	0.693	0.718	0.886	1.167	1.560
278.15	50.0	0.796	0.747	0.716	0.701	0.731	0.912	1.209	1.618
283.15	50.0	0.796	0.748	0.719	0.706	0.742	0.934	1.244	1.666
288.15	50.0	0.796	0.748	0.720	0.711	0.751	0.953	1.274	1.707

Table A-4. The calculated activity coefficient, $\gamma_{\pm}$, of NaBr(aq) — Continued

		m / mol·kg^{-1}							
T/K	p/ MPa	0.1	0.25	0.5	1.0	2.0	4.0	6.0	8.0
293.15	50.0	0.795	0.748	0.722	0.714	0.758	0.968	1.299	1.740
298.15	50.0	0.794	0.748	0.722	0.716	0.764	0.981	1.319	1.765
303.15	50.0	0.793	0.747	0.722	0.718	0.769	0.991	1.335	1.785
308.15	50.0	0.792	0.746	0.722	0.718	0.772	0.999	1.347	1.798
313.15	50.0	0.791	0.745	0.721	0.719	0.774	1.005	1.355	1.805
318.15	50.0	0.789	0.743	0.719	0.718	0.775	1.008	1.360	1.807
323.15	50.0	0.788	0.742	0.718	0.717	0.775	1.010	1.361	1.805
328.15	50.0	0.786	0.740	0.716	0.716	0.775	1.010	1.360	1.799
333.15	50.0	0.784	0.737	0.714	0.714	0.773	1.009	1.356	1.789
338.15	50.0	0.782	0.735	0.711	0.711	0.771	1.006	1.350	1.775
343.15	50.0	0.780	0.733	0.709	0.709	0.769	1.002	1.342	1.758
348.15	50.0	0.778	0.730	0.706	0.706	0.765	0.997	1.332	1.739
353.15	50.0	0.775	0.727	0.703	0.702	0.762	0.991	1.320	1.717
358.15	50.0	0.773	0.724	0.700	0.699	0.757	0.983	1.306	1.693
363.15	50.0	0.771	0.721	0.696	0.695	0.752	0.975	1.291	1.667
368.15	50.0	0.768	0.718	0.692	0.691	0.747	0.966	1.275	1.640
373.15	50.0	0.765	0.715	0.689	0.686	0.742	0.956	1.258	1.611
383.15	50.0	0.760	0.708	0.681	0.677	0.729	0.934	1.220	1.549
393.15	50.0	0.754	0.701	0.672	0.667	0.715	0.910	1.178	1.485
398.15	50.0	0.751	0.697	0.667	0.661	0.708	0.897	1.157	1.451
403.15	50.0	0.748	0.693	0.663	0.655	0.700	0.883	1.135	1.417
413.15	50.0	0.742	0.685	0.653	0.644	0.684	0.855	1.089	1.348
423.15	50.0	0.735	0.676	0.643	0.631	0.668	0.826	1.042	1.279
433.15	50.0	0.728	0.668	0.633	0.618	0.650	0.795	0.994	1.210
443.15	50.0	0.721	0.658	0.622	0.605	0.631	0.764	0.945	1.141
448.15	50.0	0.717	0.654	0.616	0.598	0.622	0.748	0.921	1.107
453.15	50.0	0.714	0.649	0.610	0.591	0.612	0.732	0.897	1.073
463.15	50.0	0.706	0.639	0.599	0.577	0.593	0.700	0.848	1.007
473.15	50.0	0.698	0.629	0.586	0.562	0.573	0.667	0.800	0.942
498.15	50.0	0.676	0.601	0.554	0.522	0.520	0.584	0.681	0.787
523.15	50.0	0.651	0.571	0.519	0.480	0.466	0.502	0.568	0.644
548.15	50.0	0.623	0.537	0.480	0.435	0.409	0.420	0.461	0.516
573.15	50.0	0.591	0.498	0.436	0.386	0.350	0.341	0.362	0.402
598.15	50.0	0.552	0.453	0.387	0.332	0.290	0.266	0.274	0.307
273.15	75.0	0.799	0.750	0.719	0.704	0.734	0.907	1.189	1.564
278.15	75.0	0.799	0.752	0.723	0.710	0.745	0.932	1.229	1.624
283.15	75.0	0.799	0.753	0.725	0.715	0.755	0.953	1.264	1.675
288.15	75.0	0.799	0.753	0.727	0.719	0.763	0.970	1.294	1.718
293.15	75.0	0.798	0.753	0.728	0.722	0.770	0.985	1.318	1.753
298.15	75.0	0.797	0.752	0.728	0.724	0.775	0.997	1.338	1.780
303.15	75.0	0.796	0.752	0.728	0.725	0.779	1.007	1.354	1.801
308.15	75.0	0.795	0.750	0.727	0.726	0.782	1.014	1.366	1.816
313.15	75.0	0.794	0.749	0.726	0.726	0.784	1.020	1.374	1.825
318.15	75.0	0.792	0.748	0.725	0.725	0.785	1.023	1.379	1.829
323.15	75.0	0.791	0.746	0.723	0.724	0.785	1.025	1.381	1.828
328.15	75.0	0.789	0.744	0.721	0.723	0.784	1.025	1.380	1.823
333.15	75.0	0.787	0.742	0.719	0.721	0.783	1.023	1.376	1.814
338.15	75.0	0.785	0.739	0.717	0.718	0.781	1.021	1.371	1.802
343.15	75.0	0.783	0.737	0.714	0.716	0.778	1.017	1.363	1.786
348.15	75.0	0.781	0.734	0.711	0.713	0.775	1.012	1.353	1.768
353.15	75.0	0.779	0.732	0.708	0.710	0.771	1.005	1.342	1.747
358.15	75.0	0.776	0.729	0.705	0.706	0.767	0.998	1.329	1.724
363.15	75.0	0.774	0.726	0.702	0.702	0.762	0.990	1.314	1.700
368.15	75.0	0.772	0.723	0.698	0.698	0.757	0.981	1.298	1.673
373.15	75.0	0.769	0.720	0.695	0.694	0.752	0.972	1.281	1.645
383.15	75.0	0.764	0.713	0.687	0.685	0.739	0.950	1.245	1.586
393.15	75.0	0.758	0.706	0.679	0.675	0.726	0.927	1.205	1.523
398.15	75.0	0.755	0.702	0.674	0.669	0.719	0.914	1.184	1.490
403.15	75.0	0.752	0.699	0.670	0.664	0.712	0.901	1.162	1.457
413.15	75.0	0.746	0.691	0.661	0.653	0.696	0.874	1.118	1.391
423.15	75.0	0.740	0.683	0.651	0.641	0.680	0.846	1.072	1.323
433.15	75.0	0.734	0.674	0.641	0.628	0.663	0.816	1.025	1.256
443.15	75.0	0.727	0.666	0.630	0.615	0.645	0.786	0.978	1.189
448.15	75.0	0.723	0.661	0.625	0.609	0.636	0.771	0.955	1.156
453.15	75.0	0.720	0.657	0.620	0.602	0.627	0.755	0.931	1.123

Table A-4. The calculated activity coefficient, $\gamma_{\pm}$, of NaBr(aq) — Continued

		m / mol·kg^{-1}							
T/K	p/ MPa	0.1	0.25	0.5	1.0	2.0	4.0	6.0	8.0
463.15	75.0	0.712	0.647	0.608	0.588	0.608	0.724	0.884	1.058
473.15	75.0	0.705	0.638	0.597	0.574	0.589	0.692	0.837	0.995
498.15	75.0	0.685	0.612	0.567	0.537	0.540	0.613	0.722	0.844
523.15	75.0	0.662	0.584	0.534	0.498	0.488	0.534	0.612	0.705
548.15	75.0	0.637	0.554	0.499	0.456	0.435	0.456	0.509	0.581
573.15	75.0	0.609	0.520	0.460	0.412	0.381	0.381	0.413	0.471
598.15	75.0	0.577	0.481	0.418	0.365	0.325	0.308	0.328	0.380
273.15	100.0	0.802	0.755	0.726	0.714	0.748	0.928	1.208	1.566
278.15	100.0	0.803	0.757	0.729	0.720	0.759	0.950	1.247	1.629
283.15	100.0	0.802	0.757	0.731	0.724	0.768	0.970	1.282	1.682
288.15	100.0	0.802	0.757	0.733	0.727	0.775	0.987	1.311	1.727
293.15	100.0	0.801	0.757	0.733	0.730	0.781	1.001	1.335	1.764
298.15	100.0	0.800	0.757	0.734	0.731	0.785	1.012	1.355	1.793
303.15	100.0	0.799	0.756	0.733	0.732	0.789	1.021	1.371	1.816
308.15	100.0	0.798	0.755	0.733	0.733	0.792	1.028	1.383	1.832
313.15	100.0	0.797	0.753	0.732	0.733	0.793	1.033	1.391	1.842
318.15	100.0	0.795	0.752	0.730	0.732	0.794	1.036	1.396	1.847
323.15	100.0	0.794	0.750	0.729	0.731	0.794	1.038	1.398	1.848
328.15	100.0	0.792	0.748	0.727	0.729	0.793	1.038	1.398	1.844
333.15	100.0	0.790	0.746	0.724	0.727	0.792	1.037	1.395	1.836
338.15	100.0	0.788	0.744	0.722	0.725	0.789	1.034	1.389	1.825
343.15	100.0	0.786	0.741	0.719	0.722	0.787	1.030	1.382	1.811
348.15	100.0	0.784	0.739	0.717	0.719	0.784	1.025	1.372	1.794
353.15	100.0	0.782	0.736	0.714	0.716	0.780	1.019	1.361	1.774
358.15	100.0	0.780	0.733	0.711	0.713	0.776	1.012	1.349	1.752
363.15	100.0	0.777	0.730	0.707	0.709	0.771	1.004	1.335	1.729
368.15	100.0	0.775	0.727	0.704	0.705	0.766	0.995	1.319	1.703
373.15	100.0	0.773	0.724	0.700	0.701	0.761	0.986	1.303	1.676
383.15	100.0	0.767	0.718	0.693	0.692	0.749	0.965	1.267	1.619
393.15	100.0	0.762	0.711	0.685	0.682	0.736	0.942	1.228	1.558
398.15	100.0	0.759	0.707	0.680	0.677	0.729	0.930	1.208	1.526
403.15	100.0	0.756	0.704	0.676	0.672	0.722	0.917	1.187	1.494
413.15	100.0	0.751	0.696	0.667	0.661	0.707	0.891	1.144	1.429
423.15	100.0	0.745	0.689	0.658	0.649	0.691	0.864	1.099	1.363
433.15	100.0	0.738	0.681	0.648	0.637	0.675	0.835	1.054	1.298
443.15	100.0	0.732	0.672	0.638	0.625	0.658	0.806	1.008	1.232
448.15	100.0	0.729	0.668	0.633	0.619	0.649	0.791	0.985	1.200
453.15	100.0	0.725	0.664	0.628	0.612	0.640	0.776	0.962	1.168
463.15	100.0	0.718	0.655	0.617	0.599	0.622	0.745	0.916	1.105
473.15	100.0	0.711	0.646	0.606	0.585	0.604	0.715	0.870	1.043
498.15	100.0	0.692	0.622	0.578	0.550	0.556	0.638	0.759	0.896
523.15	100.0	0.671	0.596	0.547	0.513	0.507	0.561	0.652	0.761
548.15	100.0	0.649	0.568	0.514	0.474	0.457	0.486	0.551	0.639
573.15	100.0	0.624	0.537	0.479	0.433	0.405	0.414	0.458	0.533
598.15	100.0	0.595	0.502	0.440	0.389	0.353	0.343	0.373	0.445

Table A-5. The calculated osmotic coefficient, ϕ, of NaBr(aq)

		m / mol·kg^{-1}							
T/K	p/ MPa	0.1	0.25	0.5	1.0	2.0	4.0	6.0	8.0
273.15	0.1	0.937	0.927	0.926	0.937	0.988	1.150	1.343	1.541
278.15	0.1	0.938	0.929	0.930	0.944	0.999	1.164	1.355	1.545
283.15	0.1	0.938	0.931	0.933	0.949	1.007	1.176	1.364	1.548
288.15	0.1	0.938	0.932	0.935	0.954	1.015	1.186	1.372	1.551
293.15	0.1	0.939	0.933	0.937	0.957	1.021	1.194	1.379	1.553
298.15	0.1	0.939	0.933	0.938	0.960	1.026	1.200	1.384	1.553
303.15	0.1	0.938	0.934	0.939	0.963	1.031	1.206	1.388	1.553
308.15	0.1	0.938	0.934	0.940	0.965	1.034	1.211	1.391	1.552
313.15	0.1	0.938	0.934	0.941	0.966	1.037	1.214	1.393	1.550

Table A-5. The calculated osmotic coefficient, ϕ, of NaBr(aq) — Continued

		m / mol·kg^{-1}							
T/K	p/ MPa	0.1	0.25	0.5	1.0	2.0	4.0	6.0	8.0
318.15	0.1	0.937	0.933	0.941	0.967	1.039	1.217	1.394	1.548
323.15	0.1	0.937	0.933	0.941	0.968	1.041	1.219	1.394	1.545
328.15	0.1	0.936	0.933	0.941	0.968	1.042	1.220	1.393	1.541
333.15	0.1	0.936	0.932	0.940	0.969	1.043	1.220	1.392	1.536
338.15	0.1	0.935	0.931	0.940	0.969	1.044	1.220	1.390	1.531
343.15	0.1	0.934	0.930	0.939	0.968	1.044	1.219	1.387	1.525
348.15	0.1	0.933	0.930	0.939	0.968	1.043	1.218	1.384	1.519
353.15	0.1	0.932	0.929	0.938	0.967	1.043	1.217	1.380	1.512
358.15	0.1	0.932	0.928	0.937	0.966	1.042	1.215	1.376	1.505
363.15	0.1	0.931	0.927	0.935	0.965	1.041	1.212	1.371	1.498
368.15	0.1	0.930	0.925	0.934	0.964	1.039	1.209	1.366	1.490
373.15	0.1	0.929	0.924	0.933	0.962	1.037	1.206	1.361	1.481
383.15	0.1	0.926	0.921	0.930	0.959	1.033	1.199	1.349	1.464
393.15	0.2	0.924	0.918	0.926	0.955	1.028	1.190	1.335	1.445
398.15	0.2	0.923	0.917	0.925	0.953	1.025	1.185	1.328	1.436
403.15	0.3	0.921	0.915	0.923	0.951	1.022	1.180	1.321	1.426
413.15	0.4	0.919	0.912	0.919	0.946	1.016	1.169	1.305	1.405
423.15	0.5	0.916	0.908	0.914	0.940	1.008	1.157	1.288	1.383
433.15	0.6	0.913	0.904	0.909	0.934	1.000	1.144	1.270	1.361
443.15	0.8	0.909	0.900	0.904	0.928	0.991	1.129	1.251	1.338
448.15	0.9	0.908	0.897	0.901	0.924	0.986	1.122	1.241	1.326
453.15	1.0	0.906	0.895	0.898	0.921	0.981	1.114	1.231	1.314
463.15	1.3	0.902	0.890	0.892	0.913	0.971	1.098	1.210	1.289
473.15	1.6	0.898	0.885	0.886	0.905	0.959	1.081	1.188	1.264
498.15	2.5	0.887	0.870	0.867	0.882	0.927	1.033	1.127	1.197
523.15	4.0	0.873	0.851	0.845	0.853	0.889	0.976	1.059	1.123
548.15	5.9	0.855	0.828	0.816	0.818	0.842	0.910	0.980	1.042
573.15	8.6	0.831	0.796	0.779	0.773	0.784	0.830	0.889	0.953
598.15	12.0	0.795	0.750	0.725	0.711	0.709	0.732	0.783	0.860
273.15	10.0	0.938	0.928	0.928	0.940	0.992	1.153	1.343	1.535
278.15	10.0	0.938	0.930	0.931	0.946	1.002	1.167	1.354	1.540
283.15	10.0	0.939	0.932	0.934	0.951	1.010	1.178	1.364	1.544
288.15	10.0	0.939	0.933	0.936	0.955	1.017	1.188	1.373	1.548
293.15	10.0	0.939	0.934	0.938	0.959	1.023	1.196	1.379	1.550
298.15	10.0	0.939	0.934	0.940	0.962	1.028	1.202	1.385	1.552
303.15	10.0	0.939	0.934	0.941	0.964	1.032	1.208	1.389	1.552
308.15	10.0	0.939	0.935	0.941	0.966	1.036	1.212	1.392	1.552
313.15	10.0	0.938	0.934	0.942	0.967	1.039	1.216	1.394	1.550
318.15	10.0	0.938	0.934	0.942	0.969	1.041	1.218	1.395	1.548
323.15	10.0	0.937	0.934	0.942	0.969	1.043	1.220	1.395	1.545
328.15	10.0	0.937	0.933	0.942	0.970	1.044	1.221	1.395	1.541
333.15	10.0	0.936	0.933	0.941	0.970	1.045	1.222	1.393	1.537
338.15	10.0	0.935	0.932	0.941	0.970	1.045	1.222	1.391	1.532
343.15	10.0	0.935	0.931	0.940	0.970	1.045	1.221	1.389	1.527
348.15	10.0	0.934	0.930	0.940	0.969	1.045	1.220	1.386	1.521
353.15	10.0	0.933	0.930	0.939	0.968	1.044	1.218	1.382	1.514
358.15	10.0	0.932	0.929	0.938	0.967	1.043	1.217	1.378	1.507
363.15	10.0	0.931	0.927	0.937	0.966	1.042	1.214	1.374	1.500
368.15	10.0	0.930	0.926	0.935	0.965	1.041	1.211	1.369	1.492
373.15	10.0	0.929	0.925	0.934	0.964	1.039	1.208	1.363	1.484
383.15	10.0	0.927	0.922	0.931	0.961	1.035	1.201	1.352	1.467
393.15	10.0	0.925	0.919	0.928	0.957	1.030	1.192	1.338	1.449
398.15	10.0	0.924	0.918	0.926	0.955	1.027	1.188	1.331	1.440
403.15	10.0	0.922	0.916	0.924	0.952	1.024	1.183	1.324	1.430
413.15	10.0	0.920	0.913	0.920	0.948	1.018	1.172	1.309	1.410
423.15	10.0	0.917	0.909	0.916	0.942	1.011	1.160	1.292	1.389
433.15	10.0	0.914	0.905	0.911	0.936	1.003	1.147	1.275	1.367
443.15	10.0	0.911	0.901	0.906	0.930	0.994	1.133	1.256	1.345
448.15	10.0	0.909	0.899	0.903	0.927	0.989	1.126	1.246	1.333
453.15	10.0	0.907	0.897	0.900	0.923	0.984	1.119	1.237	1.322
463.15	10.0	0.904	0.892	0.895	0.916	0.974	1.103	1.216	1.298
473.15	10.0	0.900	0.887	0.888	0.908	0.963	1.086	1.194	1.273
498.15	10.0	0.889	0.872	0.870	0.885	0.932	1.039	1.135	1.207
523.15	10.0	0.875	0.854	0.848	0.857	0.894	0.983	1.068	1.135
548.15	10.0	0.857	0.831	0.820	0.823	0.848	0.917	0.989	1.054

Table A-5. The calculated osmotic coefficient, ϕ, of NaBr(aq) — Continued

				m / mol·kg^{-1}					
T/K	p/ MPa	0.1	0.25	0.5	1.0	2.0	4.0	6.0	8.0
573.15	10.0	0.832	0.798	0.781	0.776	0.787	0.834	0.894	0.959
273.15	25.0	0.939	0.930	0.930	0.944	0.997	1.158	1.342	1.525
278.15	25.0	0.939	0.932	0.934	0.949	1.006	1.170	1.354	1.532
283.15	25.0	0.940	0.933	0.936	0.954	1.014	1.181	1.364	1.538
288.15	25.0	0.940	0.934	0.938	0.958	1.021	1.191	1.373	1.543
293.15	25.0	0.940	0.935	0.940	0.961	1.026	1.198	1.380	1.547
298.15	25.0	0.940	0.935	0.941	0.964	1.031	1.205	1.386	1.549
303.15	25.0	0.940	0.936	0.942	0.966	1.035	1.210	1.390	1.550
308.15	25.0	0.939	0.936	0.943	0.968	1.038	1.215	1.393	1.550
313.15	25.0	0.939	0.936	0.943	0.969	1.041	1.218	1.395	1.550
318.15	25.0	0.939	0.935	0.943	0.970	1.043	1.221	1.396	1.548
323.15	25.0	0.938	0.935	0.943	0.971	1.045	1.222	1.397	1.545
328.15	25.0	0.938	0.935	0.943	0.972	1.046	1.224	1.396	1.542
333.15	25.0	0.937	0.934	0.943	0.972	1.047	1.224	1.395	1.538
338.15	25.0	0.936	0.933	0.942	0.972	1.047	1.224	1.394	1.534
343.15	25.0	0.936	0.933	0.942	0.971	1.047	1.224	1.391	1.529
348.15	25.0	0.935	0.932	0.941	0.971	1.047	1.223	1.388	1.523
353.15	25.0	0.934	0.931	0.940	0.970	1.047	1.221	1.385	1.517
358.15	25.0	0.933	0.930	0.939	0.969	1.046	1.219	1.381	1.511
363.15	25.0	0.932	0.929	0.938	0.968	1.045	1.217	1.377	1.504
368.15	25.0	0.931	0.928	0.937	0.967	1.043	1.214	1.372	1.496
373.15	25.0	0.930	0.926	0.936	0.966	1.042	1.211	1.367	1.489
383.15	25.0	0.928	0.924	0.933	0.963	1.038	1.204	1.356	1.472
393.15	25.0	0.926	0.921	0.930	0.959	1.033	1.196	1.343	1.455
398.15	25.0	0.925	0.920	0.928	0.957	1.030	1.191	1.336	1.446
403.15	25.0	0.924	0.918	0.926	0.955	1.027	1.187	1.329	1.437
413.15	25.0	0.921	0.915	0.922	0.950	1.021	1.176	1.314	1.417
423.15	25.0	0.918	0.911	0.918	0.945	1.014	1.165	1.298	1.397
433.15	25.0	0.915	0.907	0.914	0.940	1.006	1.153	1.282	1.377
443.15	25.0	0.912	0.903	0.909	0.934	0.998	1.139	1.264	1.355
448.15	25.0	0.911	0.901	0.906	0.930	0.994	1.132	1.255	1.344
453.15	25.0	0.909	0.899	0.904	0.927	0.989	1.125	1.245	1.333
463.15	25.0	0.906	0.895	0.898	0.920	0.979	1.110	1.226	1.311
473.15	25.0	0.902	0.890	0.892	0.913	0.969	1.094	1.206	1.287
498.15	25.0	0.892	0.876	0.876	0.892	0.940	1.050	1.150	1.227
523.15	25.0	0.880	0.860	0.856	0.866	0.905	0.999	1.088	1.162
548.15	25.0	0.864	0.840	0.831	0.836	0.864	0.939	1.018	1.091
573.15	25.0	0.845	0.814	0.800	0.798	0.814	0.868	0.938	1.016
598.15	25.0	0.817	0.778	0.757	0.748	0.751	0.783	0.846	0.942
273.15	50.0	0.940	0.933	0.934	0.949	1.005	1.164	1.340	1.509
278.15	50.0	0.941	0.934	0.937	0.955	1.013	1.176	1.353	1.520
283.15	50.0	0.941	0.936	0.940	0.959	1.020	1.186	1.364	1.528
288.15	50.0	0.941	0.937	0.941	0.962	1.026	1.195	1.373	1.535
293.15	50.0	0.941	0.937	0.943	0.965	1.031	1.203	1.381	1.541
298.15	50.0	0.941	0.937	0.944	0.968	1.036	1.209	1.387	1.544
303.15	50.0	0.941	0.938	0.945	0.970	1.039	1.214	1.391	1.547
308.15	50.0	0.941	0.938	0.945	0.971	1.042	1.218	1.395	1.548
313.15	50.0	0.940	0.937	0.946	0.973	1.045	1.222	1.397	1.548
318.15	50.0	0.940	0.937	0.946	0.973	1.047	1.224	1.399	1.547
323.15	50.0	0.939	0.937	0.946	0.974	1.048	1.226	1.399	1.546
328.15	50.0	0.939	0.936	0.946	0.974	1.050	1.227	1.399	1.543
333.15	50.0	0.938	0.936	0.945	0.975	1.050	1.228	1.398	1.540
338.15	50.0	0.938	0.935	0.945	0.975	1.051	1.228	1.397	1.536
343.15	50.0	0.937	0.934	0.944	0.974	1.051	1.227	1.395	1.532
348.15	50.0	0.936	0.934	0.943	0.974	1.050	1.226	1.392	1.527
353.15	50.0	0.935	0.933	0.943	0.973	1.050	1.225	1.389	1.521
358.15	50.0	0.935	0.932	0.942	0.972	1.049	1.223	1.385	1.515
363.15	50.0	0.934	0.931	0.941	0.971	1.048	1.221	1.381	1.509
368.15	50.0	0.933	0.930	0.939	0.970	1.047	1.218	1.377	1.502
373.15	50.0	0.932	0.928	0.938	0.969	1.045	1.216	1.372	1.495
383.15	50.0	0.930	0.926	0.936	0.966	1.041	1.209	1.361	1.480
393.15	50.0	0.928	0.923	0.932	0.962	1.037	1.201	1.350	1.463
398.15	50.0	0.927	0.922	0.931	0.961	1.034	1.197	1.343	1.455
403.15	50.0	0.925	0.920	0.929	0.959	1.032	1.192	1.337	1.446

Table A-5. The calculated osmotic coefficient, ϕ, of NaBr(aq) — Continued

		m / mol·kg^{-1}							
T/K	p/ MPa	0.1	0.25	0.5	1.0	2.0	4.0	6.0	8.0
413.15	50.0	0.923	0.917	0.925	0.954	1.026	1.183	1.323	1.428
423.15	50.0	0.921	0.914	0.922	0.949	1.019	1.172	1.308	1.410
433.15	50.0	0.918	0.911	0.917	0.944	1.012	1.160	1.292	1.390
443.15	50.0	0.915	0.907	0.913	0.939	1.004	1.148	1.276	1.371
448.15	50.0	0.914	0.905	0.910	0.936	1.000	1.142	1.267	1.361
453.15	50.0	0.912	0.903	0.908	0.932	0.996	1.135	1.258	1.350
463.15	50.0	0.909	0.899	0.903	0.926	0.987	1.121	1.240	1.330
473.15	50.0	0.906	0.894	0.898	0.919	0.977	1.106	1.222	1.309
498.15	50.0	0.896	0.882	0.883	0.900	0.951	1.066	1.171	1.255
523.15	50.0	0.886	0.868	0.865	0.878	0.920	1.020	1.116	1.198
548.15	50.0	0.873	0.851	0.845	0.852	0.884	0.967	1.056	1.141
573.15	50.0	0.858	0.831	0.820	0.822	0.843	0.908	0.990	1.084
598.15	50.0	0.838	0.805	0.789	0.785	0.795	0.839	0.920	1.041
273.15	75.0	0.942	0.935	0.938	0.955	1.012	1.169	1.339	1.494
278.15	75.0	0.942	0.937	0.941	0.959	1.019	1.181	1.352	1.508
283.15	75.0	0.942	0.938	0.943	0.963	1.025	1.191	1.363	1.519
288.15	75.0	0.943	0.939	0.944	0.966	1.031	1.199	1.373	1.528
293.15	75.0	0.943	0.939	0.946	0.969	1.036	1.206	1.381	1.534
298.15	75.0	0.942	0.939	0.947	0.971	1.040	1.212	1.387	1.540
303.15	75.0	0.942	0.939	0.947	0.973	1.043	1.217	1.392	1.543
308.15	75.0	0.942	0.939	0.948	0.974	1.046	1.221	1.396	1.546
313.15	75.0	0.942	0.939	0.948	0.975	1.048	1.225	1.398	1.547
318.15	75.0	0.941	0.939	0.948	0.976	1.050	1.227	1.400	1.547
323.15	75.0	0.941	0.939	0.948	0.977	1.052	1.229	1.401	1.546
328.15	75.0	0.940	0.938	0.948	0.977	1.053	1.230	1.401	1.544
333.15	75.0	0.940	0.938	0.947	0.977	1.053	1.231	1.401	1.541
338.15	75.0	0.939	0.937	0.947	0.977	1.054	1.231	1.399	1.538
343.15	75.0	0.938	0.936	0.946	0.977	1.054	1.230	1.398	1.534
348.15	75.0	0.938	0.935	0.946	0.976	1.053	1.229	1.395	1.530
353.15	75.0	0.937	0.934	0.945	0.976	1.053	1.228	1.392	1.525
358.15	75.0	0.936	0.934	0.944	0.975	1.052	1.227	1.389	1.519
363.15	75.0	0.935	0.933	0.943	0.974	1.051	1.224	1.385	1.513
368.15	75.0	0.934	0.931	0.942	0.973	1.050	1.222	1.381	1.507
373.15	75.0	0.933	0.930	0.941	0.972	1.048	1.219	1.377	1.500
383.15	75.0	0.931	0.928	0.938	0.969	1.045	1.213	1.367	1.486
393.15	75.0	0.929	0.925	0.935	0.965	1.041	1.206	1.355	1.471
398.15	75.0	0.928	0.924	0.933	0.964	1.038	1.202	1.349	1.463
403.15	75.0	0.927	0.923	0.932	0.962	1.036	1.197	1.343	1.455
413.15	75.0	0.925	0.920	0.928	0.958	1.030	1.188	1.330	1.438
423.15	75.0	0.922	0.917	0.925	0.953	1.024	1.178	1.316	1.420
433.15	75.0	0.920	0.913	0.921	0.948	1.017	1.167	1.301	1.402
443.15	75.0	0.917	0.910	0.916	0.943	1.010	1.156	1.286	1.384
448.15	75.0	0.916	0.908	0.914	0.940	1.006	1.149	1.278	1.375
453.15	75.0	0.914	0.906	0.912	0.937	1.002	1.143	1.270	1.365
463.15	75.0	0.912	0.902	0.907	0.931	0.994	1.130	1.253	1.346
473.15	75.0	0.908	0.898	0.902	0.925	0.985	1.116	1.235	1.327
498.15	75.0	0.900	0.887	0.888	0.907	0.960	1.079	1.189	1.278
523.15	75.0	0.891	0.874	0.873	0.887	0.932	1.037	1.139	1.229
548.15	75.0	0.880	0.860	0.855	0.864	0.900	0.990	1.086	1.180
573.15	75.0	0.867	0.842	0.833	0.838	0.864	0.937	1.029	1.136
598.15	75.0	0.851	0.821	0.808	0.807	0.822	0.877	0.971	1.110
273.15	100.0	0.943	0.938	0.941	0.960	1.018	1.174	1.336	1.479
278.15	100.0	0.944	0.939	0.944	0.964	1.024	1.185	1.350	1.496
283.15	100.0	0.944	0.940	0.946	0.967	1.030	1.194	1.362	1.509
288.15	100.0	0.944	0.941	0.947	0.970	1.035	1.202	1.372	1.520
293.15	100.0	0.944	0.941	0.948	0.972	1.040	1.209	1.380	1.528
298.15	100.0	0.944	0.941	0.949	0.974	1.043	1.215	1.387	1.535
303.15	100.0	0.943	0.941	0.950	0.976	1.046	1.220	1.392	1.539
308.15	100.0	0.943	0.941	0.950	0.977	1.049	1.224	1.396	1.543
313.15	100.0	0.943	0.941	0.950	0.978	1.051	1.227	1.399	1.545
318.15	100.0	0.942	0.941	0.950	0.979	1.053	1.230	1.401	1.545
323.15	100.0	0.942	0.940	0.950	0.979	1.054	1.231	1.402	1.545
328.15	100.0	0.941	0.940	0.950	0.980	1.055	1.233	1.403	1.544
333.15	100.0	0.941	0.939	0.949	0.980	1.056	1.233	1.402	1.542

Table A-5. The calculated osmotic coefficient, ϕ, of NaBr(aq) – Continued

		m / mol·kg^{-1}							
T/K	p/ MPa	0.1	0.25	0.5	1.0	2.0	4.0	6.0	8.0
338.15	100.0	0.940	0.938	0.949	0.979	1.056	1.233	1.401	1.539
343.15	100.0	0.939	0.938	0.948	0.979	1.056	1.233	1.400	1.536
348.15	100.0	0.939	0.937	0.948	0.979	1.056	1.232	1.398	1.532
353.15	100.0	0.938	0.936	0.947	0.978	1.055	1.231	1.395	1.527
358.15	100.0	0.937	0.935	0.946	0.977	1.055	1.229	1.392	1.522
363.15	100.0	0.936	0.934	0.945	0.976	1.054	1.228	1.389	1.517
368.15	100.0	0.935	0.933	0.944	0.975	1.053	1.225	1.385	1.511
373.15	100.0	0.935	0.932	0.943	0.974	1.051	1.223	1.380	1.505
383.15	100.0	0.933	0.930	0.940	0.971	1.048	1.217	1.371	1.492
393.15	100.0	0.931	0.927	0.937	0.968	1.044	1.210	1.360	1.477
398.15	100.0	0.930	0.926	0.936	0.966	1.041	1.206	1.355	1.470
403.15	100.0	0.929	0.925	0.934	0.965	1.039	1.202	1.349	1.462
413.15	100.0	0.927	0.922	0.931	0.961	1.034	1.193	1.336	1.446
423.15	100.0	0.924	0.919	0.927	0.956	1.028	1.183	1.323	1.430
433.15	100.0	0.922	0.916	0.923	0.952	1.021	1.173	1.309	1.413
443.15	100.0	0.919	0.912	0.919	0.946	1.014	1.162	1.295	1.396
448.15	100.0	0.918	0.911	0.917	0.944	1.011	1.156	1.287	1.387
453.15	100.0	0.917	0.909	0.915	0.941	1.007	1.150	1.279	1.379
463.15	100.0	0.914	0.905	0.911	0.935	0.999	1.138	1.264	1.361
473.15	100.0	0.911	0.901	0.906	0.930	0.991	1.125	1.247	1.343
498.15	100.0	0.903	0.891	0.893	0.913	0.968	1.090	1.205	1.299
523.15	100.0	0.894	0.879	0.879	0.895	0.942	1.051	1.159	1.255
548.15	100.0	0.884	0.866	0.862	0.874	0.912	1.008	1.110	1.213
573.15	100.0	0.873	0.851	0.843	0.850	0.879	0.959	1.060	1.178
598.15	100.0	0.859	0.832	0.821	0.823	0.842	0.906	1.010	1.163

Table A-6. The calculated apparent molar volume of NaBr(aq), V_ϕ / cm^3·mol^{-1}

		m / mol·kg^{-1}							
T/K	p/ MPa	0.0	0.1	0.25	0.5	1.0	2.0	4.0	8.0
273.15	0.1	19.6	20.1	20.5	21.0	21.7	22.9	24.5	26.4
278.15	0.1	20.7	21.3	21.6	22.1	22.7	23.7	25.1	26.8
283.15	0.1	21.6	22.2	22.5	22.9	23.5	24.4	25.7	27.1
288.15	0.1	22.4	22.9	23.3	23.7	24.2	25.0	26.1	27.4
293.15	0.1	23.0	23.5	23.9	24.2	24.8	25.5	26.5	27.7
298.15	0.1	23.5	24.0	24.4	24.7	25.2	25.9	26.9	27.9
303.15	0.1	23.9	24.5	24.8	25.1	25.6	26.3	27.1	28.1
308.15	0.1	24.2	24.8	25.1	25.5	26.0	26.6	27.4	28.3
313.15	0.1	24.5	25.1	25.4	25.8	26.2	26.8	27.6	28.5
318.15	0.1	24.7	25.3	25.7	26.0	26.5	27.1	27.8	28.7
323.15	0.1	24.8	25.5	25.9	26.2	26.7	27.2	28.0	28.8
328.15	0.1	25.0	25.7	26.0	26.4	26.8	27.4	28.1	28.9
333.15	0.1	25.0	25.8	26.1	26.5	26.9	27.5	28.2	29.0
338.15	0.1	25.0	25.8	26.2	26.6	27.0	27.6	28.3	29.1
343.15	0.1	25.0	25.8	26.2	26.6	27.1	27.7	28.4	29.2
348.15	0.1	25.0	25.8	26.2	26.6	27.1	27.7	28.4	29.2
353.15	0.1	24.9	25.8	26.2	26.6	27.1	27.7	28.4	29.3
358.15	0.1	24.8	25.7	26.1	26.6	27.1	27.7	28.4	29.3
363.15	0.1	24.6	25.6	26.1	26.5	27.0	27.7	28.4	29.3
368.15	0.1	24.5	25.5	25.9	26.4	26.9	27.6	28.4	29.4
373.15	0.1	24.2	25.3	25.8	26.3	26.8	27.5	28.3	29.3
383.15	0.1	23.7	24.9	25.4	25.9	26.5	27.3	28.2	29.3
393.15	0.2	23.0	24.3	24.9	25.5	26.1	27.0	27.9	29.2
398.15	0.2	22.6	24.0	24.6	25.2	25.9	26.8	27.8	29.1
403.15	0.3	22.1	23.6	24.3	24.9	25.6	26.5	27.6	29.0
413.15	0.4	21.0	22.7	23.5	24.2	25.0	26.0	27.2	28.8
423.15	0.5	19.8	21.7	22.5	23.3	24.2	25.4	26.7	28.6
433.15	0.6	18.3	20.5	21.4	22.3	23.3	24.6	26.1	28.2
443.15	0.8	16.5	19.0	20.1	21.0	22.2	23.7	25.4	27.8
448.15	0.9	15.6	18.2	19.3	20.4	21.6	23.1	25.0	27.6
453.15	1.0	14.5	17.3	18.5	19.6	21.0	22.6	24.6	27.4
463.15	1.3	12.0	15.3	16.6	17.9	19.5	21.3	23.7	26.8
473.15	1.6	9.1	12.9	14.5	15.9	17.7	19.9	22.5	26.2

Table A-6. The calculated apparent molar volume of NaBr(aq), V_ϕ / cm^3·mol^{-1}

				m / mol·kg^{-1}					
T/K	p/ MPa	0.0	0.1	0.25	0.5	1.0	2.0	4.0	8.0
498.15	2.5	−0.7	4.8	7.1	9.3	11.8	15.0	18.9	24.0
523.15	4.0	−16.6	−8.0	−4.4	−1.1	2.9	7.6	13.4	21.0
523.15	4.0	−16.6	−8.0	−4.4	−1.1	2.9	7.6	13.4	21.0
548.15	5.9	−43.8	−29.5	−23.5	−18.0	−11.5	−3.9	5.2	16.5
573.15	8.6	−96.4	−69.8	−58.8	−48.6	−36.8	−23.2	−7.9	9.9
273.15	10.0	20.1	20.7	21.0	21.5	22.2	23.3	24.9	26.7
278.15	10.0	21.2	21.7	22.1	22.5	23.1	24.1	25.4	27.0
283.15	10.0	22.1	22.6	22.9	23.3	23.9	24.8	26.0	27.3
288.15	10.0	22.8	23.3	23.6	24.0	24.5	25.3	26.4	27.6
293.15	10.0	23.3	23.9	24.2	24.6	25.1	25.8	26.8	27.9
298.15	10.0	23.8	24.4	24.7	25.0	25.5	26.2	27.1	28.1
303.15	10.0	24.2	24.8	25.1	25.4	25.9	26.5	27.4	28.3
308.15	10.0	24.5	25.1	25.4	25.8	26.2	26.8	27.6	28.5
313.15	10.0	24.8	25.4	25.7	26.1	26.5	27.1	27.8	28.6
318.15	10.0	25.0	25.6	25.9	26.3	26.7	27.3	28.0	28.8
323.15	10.0	25.1	25.8	26.1	26.5	26.9	27.5	28.2	28.9
328.15	10.0	25.3	25.9	26.3	26.6	27.1	27.6	28.3	29.1
333.15	10.0	25.3	26.0	26.4	26.7	27.2	27.7	28.4	29.2
338.15	10.0	25.4	26.1	26.5	26.8	27.3	27.8	28.5	29.2
343.15	10.0	25.4	26.1	26.5	26.9	27.3	27.9	28.5	29.3
348.15	10.0	25.3	26.1	26.5	26.9	27.4	27.9	28.6	29.4
353.15	10.0	25.3	26.1	26.5	26.9	27.4	27.9	28.6	29.4
358.15	10.0	25.1	26.0	26.4	26.8	27.3	27.9	28.6	29.5
363.15	10.0	25.0	25.9	26.4	26.8	27.3	27.9	28.6	29.5
368.15	10.0	24.8	25.8	26.3	26.7	27.2	27.8	28.6	29.5
373.15	10.0	24.6	25.7	26.1	26.6	27.1	27.8	28.5	29.5
383.15	10.0	24.1	25.3	25.8	26.3	26.9	27.6	28.4	29.5
393.15	10.0	23.5	24.8	25.3	25.9	26.5	27.3	28.2	29.4
398.15	10.0	23.1	24.5	25.0	25.6	26.3	27.1	28.1	29.3
403.15	10.0	22.7	24.1	24.7	25.3	26.0	26.9	27.9	29.2
413.15	10.0	21.7	23.3	24.0	24.7	25.4	26.4	27.5	29.0
423.15	10.0	20.6	22.4	23.1	23.9	24.7	25.8	27.1	28.8
433.15	10.0	19.2	21.2	22.1	22.9	23.9	25.1	26.5	28.5
443.15	10.0	17.6	19.9	20.9	21.8	22.9	24.2	25.9	28.2
448.15	10.0	16.7	19.2	20.2	21.2	22.4	23.8	25.5	27.9
453.15	10.0	15.7	18.4	19.5	20.5	21.7	23.3	25.2	27.7
463.15	10.0	13.5	16.5	17.8	19.0	20.4	22.1	24.3	27.2
473.15	10.0	10.9	14.3	15.8	17.1	18.8	20.8	23.2	26.6
498.15	10.0	1.9	7.0	9.1	11.0	13.4	16.3	19.9	24.7
523.15	10.0	−12.5	−4.7	−1.5	1.5	5.1	9.4	14.8	21.8
523.15	10.0	−12.5	−4.7	−1.5	1.5	5.1	9.4	14.8	21.8
548.15	10.0	−37.8	−24.8	−19.4	−14.4	−8.5	−1.5	6.9	17.4
573.15	10.0	−90.7	−65.5	−55.1	−45.4	−34.2	−21.3	−6.7	10.5
273.15	25.0	20.8	21.4	21.7	22.2	22.9	23.9	25.4	27.0
278.15	25.0	21.8	22.4	22.7	23.1	23.7	24.6	25.9	27.3
283.15	25.0	22.6	23.2	23.5	23.9	24.4	25.2	26.4	27.6
288.15	25.0	23.3	23.8	24.1	24.5	25.0	25.8	26.8	27.9
293.15	25.0	23.8	24.4	24.7	25.0	25.5	26.2	27.1	28.1
298.15	25.0	24.3	24.8	25.1	25.5	25.9	26.6	27.4	28.3
303.15	25.0	24.7	25.2	25.5	25.9	26.3	26.9	27.7	28.5
308.15	25.0	25.0	25.5	25.8	26.2	26.6	27.2	27.9	28.7
313.15	25.0	25.2	25.8	26.1	26.4	26.9	27.4	28.1	28.9
318.15	25.0	25.4	26.0	26.3	26.7	27.1	27.6	28.3	29.0
323.15	25.0	25.6	26.2	26.5	26.8	27.3	27.8	28.4	29.1
328.15	25.0	25.7	26.3	26.7	27.0	27.4	27.9	28.5	29.2
333.15	25.0	25.8	26.4	26.8	27.1	27.5	28.0	28.7	29.3
338.15	25.0	25.8	26.5	26.8	27.2	27.6	28.1	28.7	29.4
343.15	25.0	25.8	26.5	26.9	27.2	27.7	28.2	28.8	29.5
348.15	25.0	25.8	26.5	26.9	27.3	27.7	28.2	28.8	29.6
353.15	25.0	25.7	26.5	26.9	27.3	27.7	28.2	28.9	29.6
358.15	25.0	25.6	26.5	26.9	27.2	27.7	28.2	28.9	29.6
363.15	25.0	25.5	26.4	26.8	27.2	27.7	28.2	28.9	29.7
368.15	25.0	25.4	26.3	26.7	27.1	27.6	28.2	28.9	29.7
373.15	25.0	25.2	26.2	26.6	27.0	27.5	28.1	28.8	29.7

Table A-6. The calculated apparent molar volume of NaBr(aq), V_ϕ / cm^3·mol^{-1} – Continued

T/K	p/ MPa	m / mol·kg^{-1}							
		0.0	0.1	0.25	0.5	1.0	2.0	4.0	8.0
383.15	25.0	24.8	25.8	26.3	26.8	27.3	27.9	28.7	29.7
393.15	25.0	24.2	25.4	25.9	26.4	27.0	27.7	28.5	29.6
398.15	25.0	23.9	25.1	25.7	26.2	26.8	27.5	28.4	29.6
403.15	25.0	23.5	24.8	25.4	25.9	26.6	27.3	28.3	29.5
413.15	25.0	22.6	24.1	24.8	25.3	26.1	26.9	28.0	29.3
423.15	25.0	21.6	23.3	24.0	24.7	25.4	26.4	27.6	29.1
433.15	25.0	20.5	22.3	23.1	23.8	24.7	25.8	27.1	28.9
443.15	25.0	19.1	21.2	22.0	22.9	23.9	25.1	26.6	28.6
448.15	25.0	18.3	20.5	21.5	22.3	23.4	24.7	26.2	28.4
453.15	25.0	17.5	19.8	20.8	21.7	22.9	24.2	25.9	28.2
463.15	25.0	15.6	18.3	19.4	20.4	21.7	23.2	25.2	27.8
473.15	25.0	13.4	16.5	17.7	18.9	20.3	22.1	24.3	27.3
498.15	25.0	6.2	10.5	12.3	14.0	15.9	18.4	21.5	25.7
523.15	25.0	−4.7	1.6	4.2	6.6	9.5	13.0	17.5	23.5
523.15	25.0	−4.7	1.6	4.2	6.6	9.5	13.0	17.5	23.5
548.15	25.0	−22.2	−12.4	−8.4	−4.7	−0.3	5.0	11.6	20.1
573.15	25.0	−52.3	−36.1	−29.4	−23.2	−15.9	−7.4	2.6	15.1
273.15	50.0	21.9	22.5	22.8	23.2	23.8	24.8	26.1	27.6
278.15	50.0	22.8	23.3	23.7	24.0	24.6	25.4	26.6	27.8
283.15	50.0	23.5	24.0	24.3	24.7	25.2	26.0	27.0	28.1
288.15	50.0	24.1	24.6	24.9	25.3	25.7	26.4	27.3	28.3
293.15	50.0	24.6	25.1	25.4	25.7	26.2	26.8	27.6	28.5
298.15	50.0	25.0	25.5	25.8	26.1	26.6	27.1	27.9	28.7
303.15	50.0	25.3	25.9	26.2	26.5	26.9	27.4	28.1	28.9
308.15	50.0	25.6	26.2	26.5	26.8	27.2	27.7	28.3	29.0
313.15	50.0	25.9	26.4	26.7	27.0	27.4	27.9	28.5	29.2
318.15	50.0	26.0	26.6	26.9	27.2	27.6	28.1	28.7	29.3
323.15	50.0	26.2	26.8	27.1	27.4	27.8	28.2	28.8	29.4
328.15	50.0	26.3	26.9	27.2	27.5	27.9	28.4	28.9	29.5
333.15	50.0	26.4	27.0	27.3	27.6	28.0	28.5	29.0	29.6
338.15	50.0	26.4	27.1	27.4	27.7	28.1	28.6	29.1	29.7
343.15	50.0	26.4	27.1	27.5	27.8	28.2	28.6	29.2	29.8
348.15	50.0	26.4	27.1	27.5	27.8	28.2	28.7	29.2	29.8
353.15	50.0	26.4	27.1	27.5	27.8	28.2	28.7	29.3	29.9
358.15	50.0	26.3	27.1	27.5	27.8	28.2	28.7	29.3	29.9
363.15	50.0	26.2	27.1	27.4	27.8	28.2	28.7	29.3	29.9
368.15	50.0	26.1	27.0	27.4	27.7	28.2	28.7	29.3	30.0
373.15	50.0	26.0	26.9	27.3	27.6	28.1	28.6	29.2	30.0
383.15	50.0	25.6	26.6	27.0	27.4	27.9	28.5	29.2	30.0
393.15	50.0	25.2	26.2	26.7	27.1	27.7	28.3	29.0	29.9
398.15	50.0	24.9	26.0	26.5	27.0	27.5	28.1	28.9	29.9
403.15	50.0	24.6	25.8	26.3	26.8	27.3	28.0	28.8	29.8
413.15	50.0	23.9	25.2	25.8	26.3	26.9	27.7	28.6	29.7
423.15	50.0	23.1	24.5	25.1	25.7	26.4	27.2	28.2	29.6
433.15	50.0	22.1	23.7	24.4	25.1	25.8	26.7	27.9	29.4
443.15	50.0	21.0	22.8	23.6	24.3	25.1	26.1	27.4	29.2
448.15	50.0	20.4	22.3	23.1	23.8	24.7	25.8	27.2	29.0
453.15	50.0	19.8	21.8	22.6	23.4	24.3	25.5	26.9	28.9
463.15	50.0	18.3	20.5	21.5	22.3	23.4	24.7	26.3	28.6
473.15	50.0	16.6	19.1	20.2	21.2	22.3	23.8	25.6	28.2
498.15	50.0	11.3	14.7	16.1	17.4	19.0	21.0	23.5	27.0
523.15	50.0	3.6	8.4	10.3	12.2	14.4	17.1	20.6	25.4
523.15	50.0	3.6	8.4	10.3	12.2	14.4	17.1	20.6	25.4
548.15	50.0	−7.4	−0.6	2.2	4.8	7.9	11.7	16.5	23.2
573.15	50.0	−23.9	−13.7	−9.6	−5.8	−1.3	4.2	11.0	20.0
273.15	75.0	22.9	23.4	23.7	24.1	24.7	25.5	26.7	28.0
278.15	75.0	23.7	24.2	24.5	24.8	25.3	26.1	27.1	28.2
283.15	75.0	24.3	24.8	25.1	25.4	25.9	26.6	27.5	28.4
288.15	75.0	24.8	25.3	25.6	25.9	26.4	27.0	27.8	28.6
293.15	75.0	25.3	25.8	26.0	26.3	26.8	27.3	28.1	28.8
298.15	75.0	25.6	26.1	26.4	26.7	27.1	27.6	28.3	29.0
303.15	75.0	25.9	26.5	26.7	27.0	27.4	27.9	28.5	29.1
308.15	75.0	26.2	26.7	27.0	27.3	27.7	28.1	28.7	29.3
313.15	75.0	26.4	27.0	27.2	27.5	27.9	28.3	28.9	29.4

Table A-6. The calculated apparent molar volume of NaBr(aq), V_ϕ / cm^3·mol^{-1} — Continued

		m / mol·kg^{-1}							
T/K	p/ MPa	0.0	0.1	0.25	0.5	1.0	2.0	4.0	8.0
328.15	75.0	26.8	27.4	27.7	28.0	28.3	28.8	29.3	29.8
333.15	75.0	26.9	27.5	27.8	28.1	28.5	28.9	29.4	29.8
338.15	75.0	27.0	27.6	27.9	28.2	28.5	29.0	29.4	29.9
343.15	75.0	27.0	27.6	27.9	28.2	28.6	29.0	29.5	30.0
348.15	75.0	27.0	27.7	28.0	28.3	28.6	29.1	29.5	30.0
353.15	75.0	27.0	27.7	28.0	28.3	28.7	29.1	29.6	30.1
358.15	75.0	26.9	27.7	28.0	28.3	28.7	29.1	29.6	30.1
363.15	75.0	26.9	27.6	28.0	28.3	28.7	29.1	29.6	30.2
368.15	75.0	26.8	27.6	27.9	28.2	28.6	29.1	29.6	30.2
373.15	75.0	26.7	27.5	27.8	28.2	28.6	29.1	29.6	30.2
383.15	75.0	26.4	27.2	27.6	28.0	28.4	28.9	29.5	30.2
393.15	75.0	26.0	26.9	27.4	27.8	28.2	28.8	29.4	30.2
398.15	75.0	25.7	26.8	27.2	27.6	28.1	28.7	29.3	30.2
403.15	75.0	25.5	26.6	27.0	27.4	27.9	28.5	29.2	30.1
413.15	75.0	24.9	26.1	26.6	27.0	27.6	28.2	29.0	30.0
423.15	75.0	24.2	25.5	26.1	26.6	27.2	27.9	28.8	29.9
433.15	75.0	23.4	24.9	25.5	26.0	26.7	27.5	28.4	29.8
443.15	75.0	22.5	24.1	24.7	25.4	26.1	27.0	28.1	29.6
448.15	75.0	22.0	23.7	24.4	25.0	25.8	26.7	27.9	29.5
453.15	75.0	21.5	23.2	23.9	24.6	25.4	26.4	27.7	29.4
463.15	75.0	20.3	22.2	23.0	23.8	24.7	25.8	27.2	29.1
473.15	75.0	19.0	21.1	22.0	22.8	23.8	25.0	26.6	28.8
498.15	75.0	14.7	17.6	18.7	19.8	21.1	22.8	24.9	27.9
523.15	75.0	9.0	12.8	14.4	15.8	17.6	19.8	22.6	26.7
523.15	75.0	9.0	12.8	14.4	15.8	17.6	19.8	22.6	26.7
548.15	75.0	1.1	6.4	8.5	10.5	12.8	15.8	19.7	25.1
573.15	75.0	−9.7	−2.4	0.6	3.3	6.6	10.6	15.7	22.9
273.15	100.0	23.8	24.2	24.5	24.9	25.4	26.2	27.3	28.4
278.15	100.0	24.4	24.9	25.2	25.5	26.0	26.7	27.6	28.6
283.15	100.0	25.0	25.5	25.7	26.1	26.5	27.1	27.9	28.8
288.15	100.0	25.5	25.9	26.2	26.5	26.9	27.5	28.2	28.9
293.15	100.0	25.9	26.3	26.6	26.9	27.3	27.8	28.5	29.1
298.15	100.0	26.2	26.7	26.9	27.2	27.6	28.1	28.7	29.3
303.15	100.0	26.5	27.0	27.2	27.5	27.9	28.3	28.9	29.4
308.15	100.0	26.7	27.2	27.5	27.8	28.1	28.5	29.0	29.5
313.15	100.0	26.9	27.4	27.7	28.0	28.3	28.7	29.2	29.7
318.15	100.0	27.1	27.6	27.9	28.1	28.5	28.9	29.3	29.8
323.15	100.0	27.2	27.8	28.0	28.3	28.6	29.0	29.5	29.9
328.15	100.0	27.3	27.9	28.2	28.4	28.7	29.1	29.6	30.0
333.15	100.0	27.4	28.0	28.3	28.5	28.8	29.2	29.7	30.0
338.15	100.0	27.5	28.1	28.3	28.6	28.9	29.3	29.7	30.1
343.15	100.0	27.5	28.1	28.4	28.7	29.0	29.4	29.8	30.2
348.15	100.0	27.5	28.1	28.4	28.7	29.0	29.4	29.8	30.2
353.15	100.0	27.5	28.1	28.4	28.7	29.1	29.5	29.9	30.3
358.15	100.0	27.5	28.1	28.4	28.7	29.1	29.5	29.9	30.3
363.15	100.0	27.4	28.1	28.4	28.7	29.1	29.5	29.9	30.4
368.15	100.0	27.3	28.1	28.4	28.7	29.0	29.5	29.9	30.4
373.15	100.0	27.2	28.0	28.3	28.6	29.0	29.4	29.9	30.4
383.15	100.0	27.0	27.8	28.2	28.5	28.9	29.3	29.8	30.4
393.15	100.0	26.7	27.6	27.9	28.3	28.7	29.2	29.8	30.4
398.15	100.0	26.5	27.4	27.8	28.2	28.6	29.1	29.7	30.4
403.15	100.0	26.3	27.2	27.6	28.0	28.5	29.0	29.6	30.4
413.15	100.0	25.8	26.8	27.3	27.7	28.2	28.7	29.4	30.3
423.15	100.0	25.2	26.3	26.8	27.3	27.8	28.4	29.2	30.2
433.15	100.0	24.5	25.8	26.3	26.8	27.4	28.1	28.9	30.1
443.15	100.0	23.7	25.1	25.7	26.2	26.9	27.7	28.6	29.9
448.15	100.0	23.3	24.8	25.4	25.9	26.6	27.4	28.4	29.8
453.15	100.0	22.8	24.4	25.0	25.6	26.3	27.2	28.3	29.7
463.15	100.0	21.9	23.5	24.2	24.9	25.7	26.6	27.8	29.5
473.15	100.0	20.7	22.6	23.4	24.1	24.9	26.0	27.4	29.3
498.15	100.0	17.3	19.7	20.7	21.6	22.7	24.1	26.0	28.6
523.15	100.0	12.8	15.9	17.2	18.4	19.9	21.7	24.1	27.7
523.15	100.0	12.8	15.9	17.2	18.4	19.9	21.7	24.1	27.7
548.15	100.0	6.8	11.0	12.7	14.3	16.2	18.6	21.8	26.4
573.15	100.0	−1.0	4.6	6.9	9.0	11.5	14.7	18.8	24.8

Table A-7. The calculated density of NaBr(aq). Units are kg·m^{-3}

		m / mol·kg^{-1}							
T/K	*p*/ MPa	0.0	0.1	0.25	0.5	1.0	2.0	4.0	8.0
273.15	0.1	999.844	1008.10	1020.33	1040.36	1079.26	1152.91	1285.42	1504.91
278.15	0.1	999.970	1008.11	1020.17	1039.94	1078.35	1151.16	1282.62	1501.52
283.15	0.1	999.705	1007.76	1019.68	1039.22	1077.22	1149.32	1279.83	1497.97
288.15	0.1	999.103	1007.08	1018.88	1038.24	1075.88	1147.37	1277.01	1494.31
293.15	0.1	998.204	1006.11	1017.82	1037.01	1074.35	1145.31	1274.16	1490.59
298.15	0.1	997.041	1004.89	1016.51	1035.57	1072.64	1143.13	1271.26	1486.80
303.15	0.1	995.641	1003.44	1014.99	1033.92	1070.76	1140.82	1268.31	1482.97
308.15	0.1	994.023	1001.78	1013.26	1032.09	1068.72	1138.41	1265.29	1479.11
313.15	0.1	992.206	999.92	1011.35	1030.08	1066.53	1135.88	1262.21	1475.21
318.15	0.1	990.203	997.89	1009.26	1027.90	1064.19	1133.23	1259.06	1471.29
323.15	0.1	988.026	995.68	1007.01	1025.58	1061.71	1130.49	1255.85	1467.34
328.15	0.1	985.686	993.32	1004.60	1023.10	1059.11	1127.63	1252.58	1463.36
333.15	0.1	983.192	990.80	1002.05	1020.49	1056.38	1124.68	1249.24	1459.36
338.15	0.1	980.549	988.14	999.36	1017.74	1053.53	1121.63	1245.84	1455.33
343.15	0.1	977.766	985.34	996.53	1014.87	1050.56	1118.48	1242.37	1451.27
348.15	0.1	974.847	982.40	993.57	1011.87	1047.47	1115.24	1238.84	1447.18
353.15	0.1	971.798	979.34	990.49	1008.75	1044.28	1111.90	1235.25	1443.07
358.15	0.1	968.621	976.16	987.29	1005.52	1040.99	1108.48	1231.59	1438.93
363.15	0.1	965.322	972.85	983.97	1002.17	1037.58	1104.97	1227.88	1434.76
368.15	0.1	961.903	969.42	980.53	998.71	1034.08	1101.37	1224.10	1430.55
373.15	0.1	958.367	965.89	976.98	995.15	1030.48	1097.69	1220.26	1426.32
383.15	0.1	950.970	958.49	969.57	987.72	1023.00	1090.10	1212.43	1417.77
393.15	0.2	943.132	950.66	961.75	979.89	1015.15	1082.19	1204.37	1409.10
398.15	0.2	939.051	946.58	957.68	975.82	1011.08	1078.12	1200.26	1404.71
403.15	0.3	934.864	942.40	953.51	971.66	1006.93	1073.98	1196.09	1400.29
413.15	0.4	926.169	933.73	944.86	963.04	998.35	1065.46	1187.60	1391.35
423.15	0.5	917.049	924.64	935.81	954.04	989.42	1056.64	1178.89	1382.28
433.15	0.6	907.499	915.14	926.35	944.64	980.14	1047.52	1169.98	1373.07
443.15	0.8	897.510	905.20	916.47	934.86	970.50	1038.11	1160.87	1363.74
448.15	0.9	892.347	900.07	911.38	929.81	965.54	1033.30	1156.24	1359.02
453.15	1.0	887.069	894.82	906.17	924.67	960.49	1028.41	1151.57	1354.27
463.15	1.3	876.159	883.99	895.43	914.06	950.11	1018.41	1142.07	1344.68
473.15	1.6	864.756	872.68	884.24	903.03	939.36	1008.10	1132.40	1334.96
498.15	2.5	833.879	842.12	854.07	873.41	910.69	980.99	1107.45	1310.12
523.15	4.0	799.045	807.78	820.32	840.52	879.25	951.90	1081.54	1284.45
523.15	4.0	799.045	807.78	820.32	840.52	879.25	951.90	1081.54	1284.45
548.15	5.9	759.142	768.67	782.16	803.70	844.65	920.80	1054.99	1257.71
573.15	8.6	712.233	723.16	738.28	762.07	806.65	888.20	1028.58	1228.99
273.15	10.0	1004.822	1013.06	1025.25	1045.23	1084.03	1157.45	1289.56	1508.47
278.15	10.0	1004.783	1012.91	1024.94	1044.66	1082.99	1155.62	1286.73	1505.09
283.15	10.0	1004.386	1012.42	1024.32	1043.83	1081.75	1153.70	1283.90	1501.57
288.15	10.0	1003.676	1011.64	1023.43	1042.75	1080.33	1151.69	1281.07	1497.94
293.15	10.0	1002.692	1010.59	1022.28	1041.45	1078.74	1149.58	1278.20	1494.24
298.15	10.0	1001.461	1009.30	1020.91	1039.94	1076.97	1147.36	1275.29	1490.49
303.15	10.0	1000.008	1007.80	1019.34	1038.25	1075.05	1145.03	1272.33	1486.69
308.15	10.0	998.351	1006.10	1017.57	1036.38	1072.98	1142.59	1269.31	1482.86
313.15	10.0	996.506	1004.22	1015.63	1034.35	1070.76	1140.04	1266.23	1478.99
318.15	10.0	994.486	1002.17	1013.53	1032.16	1068.42	1137.40	1263.09	1475.10
323.15	10.0	992.302	999.95	1011.27	1029.83	1065.94	1134.65	1259.90	1471.18
328.15	10.0	989.962	997.59	1008.87	1027.35	1063.34	1131.81	1256.64	1467.24
333.15	10.0	987.476	995.08	1006.32	1024.75	1060.61	1128.87	1253.32	1463.27
338.15	10.0	984.849	992.43	1003.64	1022.02	1057.78	1125.83	1249.94	1459.28
343.15	10.0	982.089	989.65	1000.84	1019.17	1054.83	1122.71	1246.50	1455.26
348.15	10.0	979.199	986.75	997.91	1016.20	1051.78	1119.49	1243.00	1451.21
353.15	10.0	976.184	983.72	994.86	1013.11	1048.62	1116.19	1239.44	1447.14
358.15	10.0	973.049	980.58	991.70	1009.92	1045.36	1112.81	1235.83	1443.03
363.15	10.0	969.797	977.32	988.42	1006.62	1042.00	1109.34	1232.15	1438.90
368.15	10.0	966.431	973.94	985.04	1003.21	1038.55	1105.79	1228.42	1434.74
373.15	10.0	962.953	970.46	981.55	999.70	1035.00	1102.16	1224.63	1430.55
383.15	10.0	955.671	963.18	974.25	992.38	1027.62	1094.66	1216.88	1422.08
393.15	10.0	947.964	955.48	966.55	984.67	1019.88	1086.86	1208.90	1413.47
398.15	10.0	943.954	951.47	962.55	980.67	1015.88	1082.84	1204.83	1409.12
403.15	10.0	939.841	947.36	958.45	976.57	1011.79	1078.75	1200.71	1404.73
413.15	10.0	931.306	938.85	949.95	968.10	1003.35	1070.35	1192.30	1395.85
423.15	10.0	922.357	929.93	941.06	959.25	994.56	1061.65	1183.68	1386.82

Table A-7. The calculated density of NaBr(aq). Units are kg·m^{-3} — Continued

		m / mol·kg^{-1}							
T/K	p/ MPa	0.0	0.1	0.25	0.5	1.0	2.0	4.0	8.0
433.15	10.0	912.988	920.60	931.77	950.02	985.42	1052.65	1174.84	1377.64
443.15	10.0	903.189	910.84	922.07	940.39	975.93	1043.36	1165.80	1368.32
448.15	10.0	898.123	905.81	917.07	935.43	971.04	1038.59	1161.20	1363.60
453.15	10.0	892.944	900.66	911.95	930.37	966.06	1033.76	1156.54	1358.85
463.15	10.0	882.230	890.01	901.39	919.93	955.82	1023.85	1147.07	1349.22
473.15	10.0	871.019	878.88	890.36	909.04	945.19	1013.62	1137.40	1339.44
498.15	10.0	840.555	848.71	860.53	879.71	916.71	986.55	1112.27	1314.30
523.15	10.0	805.848	814.45	826.82	846.78	885.11	957.11	1085.81	1288.10
523.15	10.0	805.848	814.45	826.82	846.78	885.11	957.11	1085.81	1288.10
548.15	10.0	765.271	774.62	787.88	809.10	849.54	924.89	1058.05	1260.57
573.15	10.0	715.397	726.16	741.10	764.62	808.79	889.75	1029.54	1230.48
273.15	25.0	1012.149	1020.35	1032.50	1052.40	1091.05	1164.17	1295.72	1513.83
278.15	25.0	1011.876	1019.98	1031.98	1051.63	1089.83	1162.20	1292.83	1510.48
283.15	25.0	1011.288	1019.31	1031.18	1050.63	1088.45	1160.18	1289.97	1506.99
288.15	25.0	1010.425	1018.37	1030.13	1049.41	1086.91	1158.08	1287.10	1503.40
293.15	25.0	1009.316	1017.20	1028.87	1048.00	1085.21	1155.90	1284.20	1499.73
298.15	25.0	1007.986	1015.81	1027.41	1046.41	1083.37	1153.62	1281.27	1496.02
303.15	25.0	1006.455	1014.24	1025.76	1044.64	1081.39	1151.25	1278.30	1492.26
308.15	25.0	1004.739	1012.48	1023.94	1042.72	1079.27	1148.78	1275.28	1488.47
313.15	25.0	1002.852	1010.56	1021.96	1040.65	1077.03	1146.21	1272.20	1484.65
318.15	25.0	1000.804	1008.48	1019.83	1038.44	1074.66	1143.56	1269.08	1480.80
323.15	25.0	998.605	1006.25	1017.56	1036.10	1072.17	1140.81	1265.90	1476.93
328.15	25.0	996.264	1003.88	1015.15	1033.62	1069.57	1137.98	1262.66	1473.03
333.15	25.0	993.786	1001.38	1012.62	1031.03	1066.86	1135.05	1259.37	1469.11
338.15	25.0	991.179	998.75	1009.96	1028.32	1064.05	1132.04	1256.02	1465.17
343.15	25.0	988.447	996.00	1007.18	1025.50	1061.13	1128.95	1252.62	1461.21
348.15	25.0	985.595	993.14	1004.29	1022.56	1058.12	1125.78	1249.17	1457.22
353.15	25.0	982.627	990.16	1001.29	1019.52	1055.00	1122.52	1245.66	1453.20
358.15	25.0	979.547	987.07	998.18	1016.38	1051.80	1119.19	1242.09	1449.16
363.15	25.0	976.359	983.87	994.96	1013.14	1048.50	1115.78	1238.47	1445.09
368.15	25.0	973.064	980.57	991.65	1009.80	1045.11	1112.29	1234.80	1440.99
373.15	25.0	969.665	977.16	988.24	1006.37	1041.63	1108.73	1231.08	1436.87
383.15	25.0	962.566	970.06	981.12	999.22	1034.43	1101.39	1223.47	1428.53
393.15	25.0	955.075	962.57	973.62	991.71	1026.88	1093.77	1215.66	1420.06
398.15	25.0	951.185	958.68	969.74	987.83	1022.99	1089.85	1211.67	1415.78
403.15	25.0	947.201	954.70	965.76	983.85	1019.01	1085.87	1207.64	1411.47
413.15	25.0	938.951	946.47	957.54	975.65	1010.83	1077.69	1199.42	1402.74
423.15	25.0	930.326	937.87	948.96	967.10	1002.32	1069.24	1191.00	1393.86
433.15	25.0	921.326	928.90	940.02	958.20	993.50	1060.53	1182.39	1384.85
443.15	25.0	911.943	919.55	930.72	948.96	984.36	1051.54	1173.58	1375.69
448.15	25.0	907.106	914.74	925.93	944.21	979.66	1046.95	1169.10	1371.05
453.15	25.0	902.169	909.82	921.05	939.37	974.89	1042.28	1164.57	1366.38
463.15	25.0	891.991	899.70	911.00	929.41	965.09	1032.75	1155.38	1356.92
473.15	25.0	881.391	889.17	900.54	919.07	954.95	1022.93	1145.98	1347.31
498.15	25.0	852.879	860.88	872.53	891.45	928.01	997.10	1121.65	1322.62
523.15	25.0	821.037	829.38	841.44	860.95	898.51	969.26	1096.08	1296.97
523.15	25.0	821.037	829.38	841.44	860.95	898.51	969.26	1096.08	1296.97
548.15	25.0	784.971	793.82	806.50	826.89	865.93	939.08	1069.21	1270.38
573.15	25.0	743.133	752.80	766.43	788.16	829.42	906.08	1040.93	1242.93
273.15	50.0	1023.813	1031.97	1044.06	1063.84	1102.26	1174.92	1305.67	1522.70
278.15	50.0	1023.193	1031.26	1043.20	1062.77	1100.78	1172.77	1302.70	1519.37
283.15	50.0	1022.318	1030.31	1042.13	1061.51	1099.17	1170.59	1299.77	1515.90
288.15	50.0	1021.219	1029.14	1040.87	1060.08	1097.45	1168.35	1296.84	1512.35
293.15	50.0	1019.917	1027.78	1039.42	1058.50	1095.60	1166.05	1293.90	1508.73
298.15	50.0	1018.431	1026.24	1037.81	1056.76	1093.64	1163.68	1290.94	1505.06
303.15	50.0	1016.776	1024.54	1036.04	1054.89	1091.56	1161.24	1287.94	1501.36
308.15	50.0	1014.964	1022.69	1034.13	1052.88	1089.37	1158.72	1284.91	1497.62
313.15	50.0	1013.006	1020.70	1032.08	1050.75	1087.07	1156.12	1281.84	1493.86
318.15	50.0	1010.909	1018.57	1029.91	1048.50	1084.66	1153.45	1278.72	1490.08
323.15	50.0	1008.682	1016.31	1027.61	1046.13	1082.16	1150.70	1275.56	1486.27
328.15	50.0	1006.330	1013.94	1025.20	1043.65	1079.56	1147.87	1272.36	1482.44
333.15	50.0	1003.859	1011.45	1022.67	1041.07	1076.86	1144.97	1269.11	1478.60
338.15	50.0	1001.274	1008.84	1020.03	1038.38	1074.08	1141.99	1265.81	1474.73
343.15	50.0	998.579	1006.13	1017.29	1035.59	1071.20	1138.95	1262.46	1470.85
348.15	50.0	995.778	1003.31	1014.45	1032.71	1068.23	1135.83	1259.07	1466.94

Table A-7. The calculated density of NaBr(aq). Units are kg·m^{-3} — Continued

		m / mol·kg^{-1}							
T/K	p/ MPa	0.0	0.1	0.25	0.5	1.0	2.0	4.0	8.0
353.15	50.0	992.874	1000.39	1011.51	1029.73	1065.18	1132.64	1255.63	1463.01
358.15	50.0	989.870	997.38	1008.48	1026.67	1062.05	1129.38	1252.14	1459.06
363.15	50.0	986.770	994.27	1005.35	1023.51	1058.84	1126.05	1248.61	1455.09
368.15	50.0	983.575	991.07	1002.13	1020.27	1055.54	1122.66	1245.03	1451.09
373.15	50.0	980.288	987.77	998.83	1016.94	1052.17	1119.20	1241.40	1447.07
383.15	50.0	973.446	980.92	991.96	1010.04	1045.20	1112.09	1234.01	1438.95
393.15	50.0	966.258	973.73	984.76	1002.82	1037.94	1104.73	1226.44	1430.71
398.15	50.0	962.538	970.01	981.04	999.10	1034.20	1100.96	1222.59	1426.55
403.15	50.0	958.734	966.21	977.24	995.29	1030.39	1097.13	1218.69	1422.36
413.15	50.0	950.882	958.37	969.41	987.46	1022.56	1089.28	1210.76	1413.88
423.15	50.0	942.708	950.21	961.26	979.34	1014.45	1081.20	1202.65	1405.28
433.15	50.0	934.212	941.74	952.81	970.91	1006.08	1072.89	1194.37	1396.53
443.15	50.0	925.396	932.95	944.05	962.20	997.43	1064.34	1185.92	1387.65
448.15	50.0	920.868	928.44	939.56	957.73	993.01	1059.98	1181.63	1383.16
453.15	50.0	916.257	923.84	934.99	953.19	988.51	1055.57	1177.30	1378.63
463.15	50.0	906.790	914.42	925.61	943.88	979.32	1046.56	1168.50	1369.46
473.15	50.0	896.986	904.66	915.91	934.27	969.85	1037.32	1159.54	1360.14
498.15	50.0	870.931	878.77	890.22	908.85	944.91	1013.16	1136.38	1336.20
523.15	50.0	842.458	850.52	862.25	881.28	918.03	987.42	1112.14	1311.35
523.15	50.0	842.458	850.52	862.25	881.28	918.03	987.42	1112.14	1311.35
548.15	50.0	811.184	819.57	831.68	851.27	888.97	959.91	1086.76	1285.68
573.15	50.0	776.540	785.37	798.01	818.33	857.28	930.27	1060.05	1259.53
273.15	75.0	1034.845	1042.97	1054.99	1074.67	1112.89	1185.17	1315.24	1531.44
278.15	75.0	1033.925	1041.96	1053.85	1073.34	1111.19	1182.86	1312.20	1528.09
283.15	75.0	1032.799	1040.76	1052.55	1071.86	1109.39	1180.53	1309.20	1524.63
288.15	75.0	1031.488	1039.39	1051.08	1070.25	1107.50	1178.17	1306.22	1521.09
293.15	75.0	1030.011	1037.86	1049.47	1068.50	1105.51	1175.77	1303.23	1517.50
298.15	75.0	1028.382	1036.18	1047.72	1066.64	1103.43	1173.31	1300.23	1513.86
303.15	75.0	1026.611	1034.37	1045.84	1064.66	1101.26	1170.80	1297.21	1510.19
308.15	75.0	1024.708	1032.42	1043.85	1062.57	1099.00	1168.23	1294.16	1506.49
313.15	75.0	1022.680	1030.36	1041.74	1060.38	1096.65	1165.60	1291.08	1502.77
318.15	75.0	1020.533	1028.19	1039.51	1058.08	1094.21	1162.90	1287.97	1499.03
323.15	75.0	1018.274	1025.90	1037.19	1055.69	1091.68	1160.14	1284.82	1495.28
328.15	75.0	1015.907	1023.51	1034.76	1053.20	1089.08	1157.31	1281.64	1491.51
333.15	75.0	1013.435	1021.01	1032.23	1050.61	1086.39	1154.43	1278.42	1487.72
338.15	75.0	1010.864	1018.42	1029.61	1047.94	1083.62	1151.48	1275.16	1483.92
343.15	75.0	1008.195	1015.74	1026.90	1045.18	1080.77	1148.46	1271.86	1480.10
348.15	75.0	1005.432	1012.96	1024.09	1042.34	1077.84	1145.39	1268.52	1476.27
353.15	75.0	1002.578	1010.09	1021.20	1039.41	1074.84	1142.25	1265.14	1472.42
358.15	75.0	999.635	1007.14	1018.23	1036.41	1071.77	1139.05	1261.72	1468.55
363.15	75.0	996.606	1004.10	1015.17	1033.32	1068.63	1135.80	1258.26	1464.66
368.15	75.0	993.493	1000.98	1012.04	1030.16	1065.41	1132.48	1254.76	1460.76
373.15	75.0	990.298	997.77	1008.82	1026.92	1062.13	1129.11	1251.22	1456.83
383.15	75.0	983.668	991.13	1002.16	1020.22	1055.36	1122.20	1244.02	1448.91
393.15	75.0	976.730	984.19	995.21	1013.25	1048.33	1115.06	1236.66	1440.89
398.15	75.0	973.148	980.61	991.62	1009.65	1044.72	1111.41	1232.92	1436.84
403.15	75.0	969.494	976.95	987.97	1005.99	1041.05	1107.71	1229.14	1432.77
413.15	75.0	961.968	969.43	980.45	998.47	1033.52	1100.15	1221.47	1424.54
423.15	75.0	954.159	961.64	972.66	990.69	1025.75	1092.38	1213.64	1416.19
433.15	75.0	946.072	953.56	964.60	982.66	1017.74	1084.41	1205.66	1407.72
443.15	75.0	937.709	945.22	956.28	974.37	1009.50	1076.23	1197.53	1399.11
448.15	75.0	933.425	940.95	952.02	970.13	1005.29	1072.07	1193.41	1394.76
453.15	75.0	929.072	936.61	947.70	965.83	1001.02	1067.86	1189.25	1390.38
463.15	75.0	920.159	927.73	938.86	957.03	992.32	1059.29	1180.81	1381.51
473.15	75.0	910.969	918.58	929.75	947.99	983.38	1050.52	1172.22	1372.49
498.15	75.0	886.745	894.47	905.79	924.24	959.99	1027.71	1150.10	1349.33
523.15	75.0	860.646	868.54	880.06	898.80	935.06	1003.60	1127.03	1325.28
523.15	75.0	860.646	868.54	880.06	898.80	935.06	1003.60	1127.03	1325.28
548.15	75.0	832.494	840.61	852.40	871.53	908.45	978.09	1102.96	1300.41
573.15	75.0	802.045	810.45	822.58	842.19	879.93	950.93	1077.73	1275.04
273.15	100.0	1045.296	1053.38	1065.35	1084.95	1123.00	1194.94	1324.45	1540.00
278.15	100.0	1044.119	1052.13	1063.98	1083.39	1121.10	1192.49	1321.34	1536.62
283.15	100.0	1042.774	1050.71	1062.47	1081.72	1119.13	1190.03	1318.28	1533.14
288.15	100.0	1041.277	1049.16	1060.82	1079.94	1117.09	1187.56	1315.23	1529.60
293.15	100.0	1039.644	1047.47	1059.06	1078.06	1114.98	1185.07	1312.19	1526.00

Table A-7. The calculated density of NaBr(aq). Units are kg·m^{-3} — Continued

		m / mol·kg^{-1}							
T/K	p/ MPa	0.0	0.1	0.25	0.5	1.0	2.0	4.0	8.0
298.15	100.0	1037.883	1045.67	1057.19	1076.08	1112.80	1182.53	1309.15	1522.37
303.15	100.0	1036.005	1043.75	1055.21	1074.00	1110.54	1179.95	1306.10	1518.72
308.15	100.0	1034.016	1041.72	1053.13	1071.83	1108.21	1177.33	1303.03	1515.04
313.15	100.0	1031.921	1039.60	1050.96	1069.58	1105.81	1174.66	1299.94	1511.34
318.15	100.0	1029.726	1037.37	1048.69	1067.24	1103.33	1171.94	1296.82	1507.64
323.15	100.0	1027.433	1035.05	1046.33	1064.82	1100.78	1169.16	1293.68	1503.92
328.15	100.0	1025.047	1032.64	1043.88	1062.31	1098.16	1166.33	1290.51	1500.18
333.15	100.0	1022.570	1030.14	1041.35	1059.72	1095.47	1163.45	1287.31	1496.44
338.15	100.0	1020.005	1027.56	1038.74	1057.06	1092.71	1160.52	1284.08	1492.69
343.15	100.0	1017.355	1024.89	1036.04	1054.32	1089.89	1157.53	1280.81	1488.93
348.15	100.0	1014.622	1022.14	1033.27	1051.51	1086.99	1154.49	1277.51	1485.15
353.15	100.0	1011.808	1019.32	1030.42	1048.62	1084.04	1151.40	1274.18	1481.37
358.15	100.0	1008.914	1016.41	1027.50	1045.66	1081.01	1148.26	1270.82	1477.57
363.15	100.0	1005.944	1013.43	1024.50	1042.64	1077.93	1145.06	1267.42	1473.75
368.15	100.0	1002.899	1010.37	1021.43	1039.54	1074.78	1141.81	1263.99	1469.93
373.15	100.0	999.780	1007.25	1018.29	1036.38	1071.57	1138.51	1260.53	1466.08
383.15	100.0	993.328	1000.78	1011.80	1029.85	1064.97	1131.77	1253.49	1458.34
393.15	100.0	986.599	994.05	1005.05	1023.08	1058.14	1124.83	1246.32	1450.52
398.15	100.0	983.134	990.58	1001.58	1019.60	1054.64	1121.28	1242.69	1446.58
403.15	100.0	979.604	987.05	998.05	1016.06	1051.09	1117.69	1239.02	1442.62
413.15	100.0	972.351	979.80	990.80	1008.80	1043.81	1110.38	1231.58	1434.62
423.15	100.0	964.848	972.31	983.31	1001.31	1036.32	1102.88	1224.00	1426.52
433.15	100.0	957.099	964.57	975.58	993.60	1028.63	1095.20	1216.29	1418.31
443.15	100.0	949.109	956.59	967.62	985.67	1020.73	1087.34	1208.44	1409.98
448.15	100.0	945.025	952.52	963.56	981.62	1016.70	1083.35	1204.47	1405.77
453.15	100.0	940.882	948.39	959.44	977.51	1012.62	1079.32	1200.47	1401.53
463.15	100.0	932.418	939.95	951.03	969.14	1004.32	1071.12	1192.35	1392.95
473.15	100.0	923.718	931.28	942.39	960.55	995.82	1062.74	1184.11	1384.24
498.15	100.0	900.930	908.58	919.81	938.14	973.68	1041.06	1162.91	1361.87
523.15	100.0	876.621	884.41	895.79	914.34	950.27	1018.28	1140.87	1338.64
523.15	100.0	876.621	884.41	895.79	914.34	950.27	1018.28	1140.87	1338.64
548.15	100.0	850.717	858.67	870.25	889.09	925.52	994.34	1117.95	1314.60
573.15	100.0	823.108	831.26	843.09	862.27	899.28	969.07	1094.01	1289.99

Table A-8. Calculated values of $\beta^{(0)}_{MX}$. Units are kg·mol^{-1}

T/K	p^a	0.1 MPa/p_w	10 MPa	25 MPa	50 MPa	75 MPa	100 MPa
268.15	0.1	0.1037	0.1060	0.1094	0.1146	0.1192	0.1233
273.15	0.1	0.1118	0.1137	0.1164	0.1205	0.1241	0.1274
278.15	0.1	0.1183	0.1198	0.1220	0.1253	0.1282	0.1308
283.15	0.1	0.1235	0.1248	0.1265	0.1292	0.1316	0.1337
288.15	0.1	0.1278	0.1289	0.1303	0.1325	0.1345	0.1362
293.15	0.1	0.1315	0.1323	0.1335	0.1353	0.1369	0.1383
298.15	0.1	0.1345	0.1352	0.1362	0.1377	0.1390	0.1401
303.15	0.1	0.1370	0.1376	0.1385	0.1397	0.1408	0.1417
308.15	0.1	0.1392	0.1397	0.1404	0.1414	0.1423	0.1430
313.15	0.1	0.1410	0.1415	0.1420	0.1429	0.1436	0.1441
318.15	0.1	0.1426	0.1429	0.1434	0.1441	0.1446	0.1451
323.15	0.1	0.1439	0.1441	0.1445	0.1451	0.1455	0.1459
328.15	0.1	0.1449	0.1452	0.1455	0.1459	0.1463	0.1465
333.15	0.1	0.1458	0.1460	0.1462	0.1466	0.1468	0.1470
338.15	0.1	0.1465	0.1466	0.1468	0.1471	0.1473	0.1474
343.15	0.1	0.1470	0.1471	0.1473	0.1475	0.1476	0.1476
348.15	0.1	0.1474	0.1475	0.1476	0.1477	0.1478	0.1478
353.15	0.1	0.1476	0.1477	0.1478	0.1479	0.1479	0.1478
358.15	0.1	0.1477	0.1478	0.1478	0.1479	0.1478	0.1477
363.15	0.1	0.1477	0.1477	0.1478	0.1478	0.1477	0.1476
368.15	0.1	0.1476	0.1476	0.1476	0.1476	0.1475	0.1473
373.15	0.1	0.1473	0.1473	0.1473	0.1473	0.1472	0.1470

Table A-8. Calculated values of $\beta^{(0)}_{MX}$. Units are kg·mol^{-1} — Continued

T/K	p^a	0.1 MPa/p_w	10 MPa	25 MPa	50 MPa	75 MPa	100 MPa
383.15	0.1	0.1466	0.1466	0.1466	0.1465	0.1463	0.1461
393.15	0.2	0.1455	0.1455	0.1454	0.1453	0.1451	0.1449
398.15	0.2	0.1448	0.1448	0.1447	0.1446	0.1444	0.1442
403.15	0.3	0.1441	0.1440	0.1440	0.1438	0.1437	0.1434
413.15	0.4	0.1423	0.1423	0.1422	0.1421	0.1419	0.1417
423.15	0.5	0.1403	0.1402	0.1402	0.1400	0.1399	0.1397
433.15	0.6	0.1380	0.1379	0.1379	0.1377	0.1376	0.1374
443.15	0.8	0.1354	0.1354	0.1353	0.1351	0.1350	0.1348
448.15	0.9	0.1340	0.1340	0.1339	0.1337	0.1336	0.1335
453.15	1.0	0.1326	0.1325	0.1324	0.1323	0.1322	0.1320
463.15	1.3	0.1294	0.1294	0.1293	0.1292	0.1291	0.1290
473.15	1.6	0.1260	0.1260	0.1259	0.1258	0.1257	0.1256
498.15	2.5	0.1163	0.1162	0.1161	0.1160	0.1159	0.1160
523.15	4.0	0.1047	0.1045	0.1042	0.1039	0.1039	0.1039
548.15	5.9	0.0907	0.0903	0.0894	0.0888	0.0885	0.0886
573.15	8.6	0.0731	0.0727	0.0702	0.0683	0.0676	0.0673
598.15	12.0	0.0483		0.0415	0.0360	0.0336	0.0325

[a] Column gives the pressure for values of $\beta^{(0)}_{MX}$ in the 0.1 MPa / p_w column.

Table A-9. Calculated values of $\beta^{(1)}_{MX}$. Units are kg·mol^{-1}

T/K	p^a	0.1 MPa/p_w	10 MPa	25 MPa	50 MPa	75 MPa	100 MPa
268.15	0.1	0.2312	0.2337	0.2375	0.2435	0.2491	0.2545
273.15	0.1	0.2521	0.2544	0.2578	0.2632	0.2684	0.2732
278.15	0.1	0.2675	0.2696	0.2727	0.2776	0.2823	0.2867
283.15	0.1	0.2794	0.2813	0.2842	0.2886	0.2929	0.2969
288.15	0.1	0.2892	0.2909	0.2935	0.2975	0.3014	0.3051
293.15	0.1	0.2975	0.2990	0.3013	0.3050	0.3085	0.3118
298.15	0.1	0.3047	0.3061	0.3082	0.3115	0.3146	0.3176
303.15	0.1	0.3112	0.3124	0.3143	0.3172	0.3201	0.3227
308.15	0.1	0.3171	0.3182	0.3199	0.3225	0.3250	0.3274
313.15	0.1	0.3226	0.3236	0.3251	0.3274	0.3296	0.3317
318.15	0.1	0.3279	0.3287	0.3300	0.3320	0.3339	0.3357
323.15	0.1	0.3329	0.3336	0.3347	0.3364	0.3380	0.3395
328.15	0.1	0.3378	0.3384	0.3393	0.3406	0.3420	0.3432
333.15	0.1	0.3426	0.3430	0.3437	0.3448	0.3458	0.3468
338.15	0.1	0.3473	0.3476	0.3481	0.3489	0.3497	0.3504
343.15	0.1	0.3519	0.3521	0.3524	0.3529	0.3534	0.3539
348.15	0.1	0.3566	0.3567	0.3568	0.3570	0.3572	0.3573
353.15	0.1	0.3612	0.3612	0.3611	0.3610	0.3609	0.3608
358.15	0.1	0.3659	0.3657	0.3655	0.3651	0.3647	0.3643
363.15	0.1	0.3707	0.3703	0.3699	0.3692	0.3685	0.3678
368.15	0.1	0.3755	0.3750	0.3744	0.3733	0.3723	0.3714
373.15	0.1	0.3803	0.3798	0.3789	0.3775	0.3762	0.3750
383.15	0.1	0.3904	0.3895	0.3882	0.3862	0.3842	0.3824
393.15	0.2	0.4009	0.3997	0.3979	0.3952	0.3926	0.3901
398.15	0.2	0.4064	0.4050	0.4030	0.3998	0.3969	0.3941
403.15	0.3	0.4120	0.4104	0.4082	0.4046	0.4013	0.3982
413.15	0.4	0.4237	0.4218	0.4190	0.4146	0.4105	0.4067
423.15	0.5	0.4361	0.4338	0.4304	0.4252	0.4203	0.4157
433.15	0.6	0.4493	0.4467	0.4426	0.4364	0.4306	0.4252
443.15	0.8	0.4635	0.4604	0.4556	0.4483	0.4415	0.4353
448.15	0.9	0.4709	0.4676	0.4624	0.4545	0.4473	0.4406
453.15	1.0	0.4786	0.4750	0.4694	0.4609	0.4532	0.4460
463.15	1.3	0.4947	0.4907	0.4842	0.4744	0.4655	0.4574
473.15	1.6	0.5121	0.5075	0.5000	0.4888	0.4786	0.4694
498.15	2.5	0.5614	0.5555	0.5448	0.5290	0.5152	0.5029
523.15	4.0	0.6209	0.6139	0.5984	0.5766	0.5580	0.5417
548.15	5.9	0.6937	0.6866	0.6635	0.6329	0.6079	0.5866
573.15	8.6	0.7847	0.7805	0.7440	0.6999	0.6663	0.6385
598.15	12.0	0.9027		0.8468	0.7805	0.7346	0.6984

[a] Column gives the pressure for values of $\beta^{(1)}_{MX}$ in the 0.1 MPa / p_w column.

Table A-10. Calculated values of $C^{(0)}_{MX}$. Units are $kg^2 \cdot mol^{-2}$

T/K	p^a	0.1 MPa/p_w	10 MPa	25 MPa	50 MPa	75 MPa	100 MPa
268.15	0.1	0.02	-0.21	-0.53	-1.03	-1.49	-1.91
273.15	0.1	-0.45	-0.62	-0.88	-1.28	-1.65	-1.99
278.15	0.1	-0.81	-0.96	-1.16	-1.49	-1.79	-2.07
283.15	0.1	-1.11	-1.23	-1.40	-1.66	-1.91	-2.14
288.15	0.1	-1.35	-1.45	-1.59	-1.81	-2.02	-2.20
293.15	0.1	-1.56	-1.64	-1.76	-1.94	-2.11	-2.27
298.15	0.1	-1.74	-1.81	-1.91	-2.06	-2.20	-2.33
303.15	0.1	-1.90	-1.95	-2.03	-2.16	-2.28	-2.38
308.15	0.1	-2.03	-2.08	-2.15	-2.25	-2.35	-2.44
313.15	0.1	-2.16	-2.19	-2.25	-2.34	-2.42	-2.49
318.15	0.1	-2.26	-2.30	-2.34	-2.41	-2.48	-2.54
323.15	0.1	-2.36	-2.39	-2.43	-2.48	-2.54	-2.58
328.15	0.1	-2.45	-2.47	-2.50	-2.55	-2.59	-2.63
333.15	0.1	-2.53	-2.55	-2.57	-2.61	-2.64	-2.67
338.15	0.1	-2.60	-2.61	-2.63	-2.66	-2.68	-2.70
343.15	0.1	-2.67	-2.68	-2.69	-2.71	-2.72	-2.74
348.15	0.1	-2.73	-2.73	-2.74	-2.75	-2.76	-2.77
353.15	0.1	-2.78	-2.78	-2.79	-2.79	-2.79	-2.79
358.15	0.1	-2.83	-2.83	-2.83	-2.83	-2.82	-2.82
363.15	0.1	-2.87	-2.87	-2.86	-2.86	-2.85	-2.84
368.15	0.1	-2.91	-2.90	-2.90	-2.88	-2.87	-2.86
373.15	0.1	-2.94	-2.93	-2.92	-2.91	-2.89	-2.88
383.15	0.1	-2.99	-2.98	-2.97	-2.94	-2.92	-2.90
393.15	0.2	-3.03	-3.02	-3.00	-2.96	-2.93	-2.90
398.15	0.2	-3.04	-3.03	-3.00	-2.97	-2.94	-2.90
403.15	0.3	-3.05	-3.03	-3.01	-2.97	-2.93	-2.90
413.15	0.4	-3.06	-3.04	-3.01	-2.96	-2.92	-2.88
423.15	0.5	-3.05	-3.02	-2.99	-2.94	-2.89	-2.85
433.15	0.6	-3.02	-3.00	-2.96	-2.90	-2.85	-2.80
443.15	0.8	-2.98	-2.95	-2.91	-2.85	-2.79	-2.74
448.15	0.9	-2.96	-2.93	-2.88	-2.81	-2.75	-2.70
453.15	1.0	-2.93	-2.90	-2.85	-2.78	-2.71	-2.66
463.15	1.3	-2.86	-2.82	-2.77	-2.69	-2.62	-2.56
473.15	1.6	-2.77	-2.73	-2.67	-2.59	-2.51	-2.45
498.15	2.5	-2.48	-2.44	-2.36	-2.25	-2.15	-2.08
523.15	4.0	-2.07	-2.02	-1.91	-1.76	-1.65	-1.55
548.15	5.9	-1.50	-1.45	-1.28	-1.08	-0.92	-0.79
573.15	8.6	-0.68	-0.65	-0.36	-0.04	0.18	0.35
598.15	12.0	0.69		1.22	1.79	2.15	2.42

Column gives the pressure for values of $C^{(0)}_{MX}$ in the 0.1 MPa / p_w column.

Table A-11. Calculated values of $C^{(1)}_{MX}$. Units are $kg^2 \cdot mol^{-2}$

T/K	p^a	0.1 MPa/p_w	10 MPa	25 MPa	50 MPa	75 MPa	100 MPa
268.15	0.1	-13.31	-13.31	-13.31	-13.31	-13.31	-13.31
273.15	0.1	-13.56	-13.56	-13.56	-13.56	-13.56	-13.56
278.15	0.1	-13.55	-13.55	-13.55	-13.55	-13.55	-13.55
283.15	0.1	-13.40	-13.40	-13.40	-13.40	-13.40	-13.40
288.15	0.1	-13.17	-13.17	-13.17	-13.17	-13.17	-13.17
293.15	0.1	-12.90	-12.90	-12.90	-12.90	-12.90	-12.90
298.15	0.1	-12.59	-12.59	-12.59	-12.59	-12.59	-12.59
303.15	0.1	-12.28	-12.28	-12.28	-12.28	-12.28	-12.28
308.15	0.1	-11.96	-11.96	-11.96	-11.96	-11.96	-11.96
313.15	0.1	-11.63	-11.63	-11.63	-11.63	-11.63	-11.63
318.15	0.1	-11.31	-11.31	-11.31	-11.31	-11.31	-11.31
323.15	0.1	-10.99	-10.99	-10.99	-10.99	-10.99	-10.99
328.15	0.1	-10.67	-10.67	-10.67	-10.67	-10.67	-10.67
333.15	0.1	-10.36	-10.36	-10.36	-10.36	-10.36	-10.36
338.15	0.1	-10.04	-10.04	-10.04	-10.04	-10.04	-10.04
343.15	0.1	-9.74	-9.74	-9.74	-9.74	-9.74	-9.74
348.15	0.1	-9.43	-9.43	-9.43	-9.43	-9.43	-9.43

Table A-11. Calculated values of $C_{MX}^{(1)}$. Units are $kg^2 \cdot mol^{-2}$ – Continued

T/K	p^a	0.1 MPa/p_w	10 MPa	25 MPa	50 MPa	75 MPa	100 MPa
353.15	0.1	−9.13	−9.13	−9.13	−9.13	−9.13	−9.13
358.15	0.1	−8.83	−8.83	−8.83	−8.83	−8.83	−8.83
363.15	0.1	−8.53	−8.53	−8.53	−8.53	−8.53	−8.53
368.15	0.1	−8.23	−8.23	−8.23	−8.23	−8.23	−8.23
373.15	0.1	−7.93	−7.93	−7.93	−7.93	−7.93	−7.93
383.15	0.1	−7.34	−7.34	−7.34	−7.34	−7.34	−7.34
393.15	0.2	−6.75	−6.75	−6.75	−6.75	−6.75	−6.75
398.15	0.2	−6.46	−6.46	−6.46	−6.46	−6.46	−6.46
403.15	0.3	−6.16	−6.16	−6.16	−6.16	−6.16	−6.16
413.15	0.4	−5.56	−5.56	−5.56	−5.56	−5.56	−5.56
423.15	0.5	−4.95	−4.95	−4.95	−4.95	−4.95	−4.95
433.15	0.6	−4.32	−4.32	−4.32	−4.32	−4.32	−4.32
443.15	0.8	−3.68	−3.68	−3.68	−3.68	−3.68	−3.68
448.15	0.9	−3.34	−3.34	−3.34	−3.34	−3.34	−3.34
453.15	1.0	−3.01	−3.01	−3.01	−3.01	−3.01	−3.01
463.15	1.3	−2.31	−2.31	−2.31	−2.31	−2.31	−2.31
473.15	1.6	−1.58	−1.58	−1.58	−1.58	−1.58	−1.58
498.15	2.5	0.47	0.47	0.47	0.47	0.47	0.47
523.15	4.0	2.96	2.96	2.96	2.96	2.96	2.96
548.15	5.9	6.25	6.25	6.25	6.25	6.25	6.25
573.15	8.6	11.15	11.15	11.15	11.15	11.15	11.15
598.15	12.0	20.10		20.10	20.10	20.10	20.10

[a] Column gives the pressure for values of $C_{MX}^{(1)}$ in the 0.1 MPa / p_w column.