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GAMPHI—A Database of Activity and Osmotic Coefficients for Aqueous Electrolyte Solutions

R. N. Goldberg, J. L. Manley, and R. L. Nuttall

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[2] Some divisions within the center are located at Boulder, CO 80303.
[3] Located at Boulder, CO, with some elements at Gaithersburg, MD.

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Abstract

A database of activity and osmotic coefficients for 350 binary aqueous electrolyte solutions at 298.15 K has been assembled together with a collection of subroutines for utilizing the database. The computer codes, which are written in FORTRAN 77, can be used either interactively or from user-written programs to calculate values of the activity and osmotic coefficients at selected molalities.

Key words: activity coefficient; database; electrolyte solutions; FORTRAN; Gibbs energy; osmotic; salts; thermodynamics; water.

1. Introduction

A database of activity ($\gamma_{\pm}$) and osmotic coefficients (ϕ) for 350 binary aqueous electrolyte solutions at 298.15 K has been assembled together with a collection of subroutines for utilizing the database. The codes, which are written in FORTRAN 77, can be used either interactively or individual subroutines can be referenced via FORTRAN CALL statements from user-written programs.

The data are contained in FORTRAN DATA statements which, for each binary electrolyte solution, contain (1) the name of the cation and anion in the binary salt, (2) the literature reference from which the data were obtained, (3) the minimum and maximum molality for which the data are valid, (4) a designation of an internal database name to which the data set belongs, (5) a designation as to whether or not the data are considered to be primary or non-primary for a given salt in the entire database, (6) an integer which indicates which equation or model is used to calculate the value of $\gamma_{\pm}$ and ϕ, (7) the number of parameters in the model, and (8) the parameters for the model. Items (4) and (5) are needed since there is frequently more than one set of data for a given salt in the entire database. The user can select whichever data set he wishes or he can simply specify the primary or default one. During execution of the program all of this information and the calculated values of $\gamma_{\pm}$ and ϕ are returned to the user.

2. Equations Used to Calculate Activity and Osmotic Coefficients

Activity and osmotic coefficients are calculated using any of several different equations. The equations used in this database, with the values of the Debye-Hückel constants which have been used in them are:

Equation 1[a]

$$\ell n\gamma_{\pm} = -A_m|z_c z_a|I^{1/2}/(1 + P_1 I^{1/2}) + \sum_{i=2}^{N} P_i m^{(i-1)}$$

$$\phi = 1 - A_m|z_c z_a|\{(1 + P_1 I^{1/2}) - 2\ \ell n(1 + P_1 I^{1/2}) - (1 + P_1 I^{1/2})\}/(P_1^3 I)$$

$$+ \sum_{i=2}^{N}[(i-1)/i]P_i m_i^{(i-1)}$$

$$A_m = 0.51084\ell n(10)$$

Equation 2

For electrolytes of charge type 2 (see table 1):

$$\ell n\gamma_{\pm} = -2A_m I^{1/2} - (2/3)A_m^2\ I\ell nI + \sum_{i=1}^{N} P_i m^{(i+1)/2}$$

$$\phi = 1 - (2/3)A_m I^{1/2} - (1/3)A_m^2 I(\ell nI + 1/2) + \sum_{i=1}^{N} \{(i + 1)/(i + 3)\}P_i m^{(i+1)/2}$$

where $A_m = 0.51084\ \ell n\ 10$

Equation 3

$$\ell n\gamma_{\pm} = -A_m|z_c z_a|I^{1/2} + \sum_{i=1}^{N} P_i m^{(i+1)/2}$$

$$\phi = 1 -(1/3)A_m|z_c z_a|I^{1/2} + \sum_{i=1}^{N}[(i+1)/(i+3)]P_i m^{(i+1)/2}$$

$$A_m = 0.51084\ell n(10)$$

---

[a] See Glossary for definitions of quantities.

Equation 4

$$\ell n \gamma_\pm = |z_c z_a| f^\gamma + B^\gamma m + (3/2)P_3 m^2$$

$$\phi = 1 + |z_c z_a| f^\phi + B^\phi m + P_3 m^2$$

$$f^\gamma = -A_\phi[I^{1/2}/(1 + bI^{1/2}) + (2/b)\ell n(1 + bI^{1/2})]$$

$$B^\gamma = 2P_1 + [2/(\alpha^2 I)]\{1 - [1 + \alpha I^{1/2} - (1/2)\alpha^2 I]\exp(-\alpha I^{1/2})\}P_2$$

$$f^\phi = -A_\phi I^{1/2}/(1 + bI^{1/2})$$

$$B^\phi = P_1 + P_2 \exp(-\alpha I^{1/2})$$

$b = 1.2$

$\alpha = 2.0$

$A_\phi = 0.391$

Equation 5

$$\ell n \gamma_\pm = |z_c z_a| f^\gamma + B^\gamma m + (3/2)P_4 m^2$$

$$\phi = 1 + |z_c z_a| f^\phi + B^\phi m + P_4 m^2$$

$$f^\gamma = -A_\phi[I^{1/2}/(1 + bI^{1/2}) + (2/b)\ell n(1 + bI^{1/2})]$$

$$B^\gamma = 2P_1 + [2/(\alpha_1^2 I)]\{1 - [1 + \alpha_1 I^{1/2} - (1/2)\alpha_1^2 I]\exp(-\alpha_1 I^{1/2})\}P_2$$

$$+ [2/(\alpha_2^2 I)]\{1 - [1 + \alpha_2 I^{1/2} - (1/2)\alpha_2^2 I]\exp(-\alpha_2 I^{1/2})\}P_3$$

$$f^\phi = -A_\phi I^{1/2}/(1 + bI^{1/2})$$

$$B^\phi = P_1 + P_2 \exp(-\alpha_1 I^{1/2}) + P_3 \exp(-\alpha_2 I^{1/2})$$

$b = 1.2$

$\alpha_1 = 1.4$

$\alpha_2 = 12.0$

$A_\phi = 0.391$

Equation 6

$$\log_{10}\gamma_{\pm} = -A|z_c z_a|I^{1/2}/(1 + P_1 I^{1/2}) + \sum_{i=2}^{N} P_i m^{(i-1)}$$

$$\phi = 1 - A\ln(10)|z_c z_a|\{(1 + P_1 I^{1/2}) - 2\ln(1 + P_1 I^{1/2})$$

$$-(1 + P_1 I^{1/2})^{-1}\}/(P_1^3 I) + \sum_{i=2}^{N} P_i[(i-1)/i]\ln(10)m^{(i-1)}$$

where A = 0.5108

Equation 7

$$\ln\gamma_{\pm} = -A|z_c z_a|I^{1/2} + \Sigma[(P_j + 1)/P_j]P_i m^{Pj}$$

$$\phi = 1 -(1/3)A|z_c z_a|I^{1/2} + \Sigma P_i m^{Pj}$$

where the summations run from i = 1, N/2 and j = (1 + N/2), N

and A = 0.5108

Equation 8

$$\ln\gamma_{\pm} = \sum_{i=1}^{N} P_i m^{i/2}$$

$$\phi = 1 + \sum_{i=1}^{N} [i/(i + 2)]P_i m^{i/2}$$

Equation 9

$$\ell n\gamma_{\pm} = |z_c z_a| f^{\gamma} + B^{\gamma} m + \sum_{i=3}^{N} P_i[i/(i-1)]m^{(i-1)}$$

$$\phi = 1 + |z_c z_a| f^{\phi} + B^{\phi} m + \sum_{i=3}^{N} P_i m^{(i-1)}$$

$$f^{\gamma} = -A_{\phi}[I^{1/2}/(1 + bI^{1/2}) + (2/b)\ell n(1 + bI^{1/2})]$$

$$B^{\gamma} = 2P_1 + [2/(\alpha^2 I)]\{ 1 - [1 + \alpha I^{1/2} - (1/2)\alpha^2 I]\exp(-\alpha I^{1/2})\}P_2$$

$$f^{\phi} = -A_{\phi} I^{1/2}/(1 + bI^{1/2})$$

$$B^{\phi} = P_1 + P_2\exp(-\alpha I^{1/2})$$

$B = 1.2$

$\alpha = 2.0$

$A_{\phi} = 0.51084\ell n(10)/3$

Equation 10

"Equation" 10 uses a piecewise cubic Hermite function [80FRI/CAR] to evaluate values of $\gamma_{\pm}$ and ϕ from discrete, tabulated values of $\gamma_{\pm}$ and ϕ as a function of molality. The subroutines which are used for the Hermite function evaluation were written by F. N. Fritsch of Lawrence Livermore Laboratory and are a part of the CMLIB collection of mathematical software [84BOI/HOW].

3. Database Designations

The internal database designations, their source(s), and the types of equations used in them are:

Designation	Reference(s)	Equation(s)
HAMWU	72HAM/WU	6
NBS1	77STA/NUT, 78GOL/NUT,79GOL/NUT, 79GOL, 81GOL, 81GOL2, 81STA	1
NBS2	" " " "	2
NBS3	" " " "	3
NBS8	81STA2	8
NBSPIT	- - - - - - - -	9
PITZER	82PEI/PIT, 79PIT, 73PIT/MAY, 74PIT/ MAY, 74PIT/PET, 77PIT/ROY, 76PIT/SIL, 78PIT/SIL	4, 5, 10
RARD	83RAR, 84RAR, 76RAR/HAB, 77RAR/HAB 81RAR/MIL, 81RAR/MIL2, 82RAR/MIL, 82RAR/MIL2, 79RAR/MIL, 77RAR/SHI, 77RAR/SPE, 81RAR/SPE,82RAR/SPE, 76SPE/WEB, 77RAR/WEB	7, 10
MISC	- - - - - - - -	---

Database NBSPIT contains values of the parameters in eq. (9) for all of the salts represented in the databases NBS1, NBS2, and NBS3. These values have not previously appeared in the literature.

In a few instances the databases contain more than one set of parameters for a given correlating equation. This can occur for example, when a new set of measurements appears in the literature. In such cases a "/0" is added to the internal database designation.

For a given salt, when there is more than one source of data, a designation of "P" (primary) has been attached to one of the data sets and a designation of "NP" attached to the remainder. While this choice is somewhat arbitrary a "P" designation has usually been attached to those data sets which cover the widest range of molality.

Database "MISC" contains those data sets which do not belong to any of the other databases and it exists primarily to accommodate future expansion of the database. If the user wishes to add additional data, it is recommended that he do so in SUBROUTINE MISC.

4. Additional Gibbs Energy Properties

Additional Gibbs energy properties of the solvent, solute, and of the solution can be calculated from the mean ionic activity coefficient and the osmotic coefficient. The properties of the solvent are:

$$a_1 = \exp(-\nu m_2 \phi / m_1^*)$$

where $m_1^* = 55.5087$ mol kg^{-1}

$$\gamma_1 = a_1 / X_1$$

where $X_1 = m_1^* / (m_2 + m_1^*)$

$$G_1^{ex} = \nu m_2 RT(1 - \phi)/m_1^*$$

$$G_1 - G_1^{o} = RT\ell n a_1 = -\nu m_2 RT\phi / m_1^*$$

The properties of the solute are:

$$\gamma_2 = \gamma_\pm^\nu$$

$$a_2 = m_2\gamma_\pm^\nu$$

$$a_\pm = m_\pm\gamma_\pm$$

where $m_\pm = (\nu_c^{\nu_c}\ \nu_a^{\nu_a})^{1/\nu}$ and $\nu = \nu_a + \nu_c$

$$G_2^{ex} = \nu RT\ell n\gamma_\pm$$

The properties of the solution are:

$$G^{ex} = \nu m_2RT(1 - \phi + \ell n\gamma_\pm)$$

$$G - G^o = \nu m_2RT[\ell n(m_2\gamma_\pm) - \phi]$$

5. Installation of Program

The GAMPHI package consists of 33 subroutines written in FORTRAN 77. Adherence to the ASNI FORTRAN standard [78AME] has been verified using the Sperry FORTRAN verifier [79SPE]. The subroutines are on a magnetic tape which is available from:

The Office of Standard Reference Data
National Bureau of Standards
Gaithersburg, MD 20899

The logical units for input and output are set in the element MAIN using the constants NIN and NOUT, respectively; the user should set their values to the appropriate ones for the computer on which the codes are being installed. No other changes to the codes should be needed. To install the interactive version, the individual subroutines must be compiled and linked together to form an executable element with the element MAIN as the principal program.

Subroutine GAMPHI can also be used directly with a CALL statement from a user-written program. For such applications, the user must link this program to all of the compiled subroutines with the exceptions of MAIN, UPPER, INTRO, TABLE, CALC, CATION, ANIONS, MENU, HELP, and SEARCH.

The source code for the GAMPHI package including the databases, requires 413 kilobytes of storage space. The memory requirement during execution of the program is 446 kilobytes.

To date, the codes have been implemented both on a VAX 11/780 and on a SPERRY (UNIVAC) 1100/82 computer. On the VAX, the codes were compiled and linked as a single element using the default options. On the SPERRY computer, the subroutines were compiled individually using the "O" option on the FTN compiler and then linked together with element MAIN as the principal program.

6. Interactive Use of Program

In the sample session which follows, the replies of the user have been underlined. Note that the replies of the user, with the exception of the specification of cations and anions, can be either upper or lower case.

```
COMMAND ("M" GIVES THE MENU)?
m

*******************MENU************************

C   CALCUALTE ACTIVITY AND OSMOTIC COEFFICIENTS
H   HELP
LA  LIST OF ANIONS IN DATABASE
LC  LIST OF CATIONS IN DATABASE
M   MENU
Q   QUIT
R   LIST OF REFERENCES TO DATABASE
S   SEARCH THE DATABASE FOR A LIST OF REFERENCES
       TO A GIVEN SALT

************************************************
```

```
COMMAND ("M" GIVES THE MENU)?
c

CATION?
Na+

ANION?
Cl-

SPECIFY DATABASE ("P" SPECIFIES PRIMARY ONE):
P

WOULD YOU LIKE A TABLE OF ACTIVITY AND OSMOTIC COEFFICIENTS (Y OR N)?
N

MOLALITY ("-1" TO STOP)?
4.52

THE CATION IS Na+
THE ANION IS Cl-
THE CHARGE TYPE OF THE SALT IS  1

    THE PRIMARY DATABASE WAS USED
    THE SELECTED MOLALITY =     4.520000 MOL/KG
    THE MIN. AND MAX. MOLALITIES ARE  .00000 AND   6.14400 MOL/KG

         ........................ .....

         ACTIVITY COEFFICIENT =    .8280
         OSMOTIC COEFFICIENT  =   1.1546

         ..............................

SEE REFERENCE 72HAM/WU

THE CALCULATION USED EQUATION NO.  6
THE   4 PARAMETERS IN THIS EQUATION ARE:

 1.44950000000000000
 .204420000000000000-001
 .579269999999999999-002
-.288600000000000000-003

MOLALITY ("-1" TO STOP)?
0.37

         ..............................

         ACTIVITY COEFFICIENT =    .6970
         OSMOTIC COEFFICIENT  =    .9202

         ..............................
```

```
MOLALITY ("-1" TO STOP)?
-1

COMMAND ("M" GIVES THE MENU)?
s

CATION (* = WILDCARD)?
Ca+2

ANION (* = WILDCARD)?
Cl-

FOR THE SALT FORMED FROM Ca+2
                     AND Cl-

DATA HAS BEEN FOUND:

REFERENCE    DATABASE    MIN.       MAX.       EQ. NO.
                           MOLALITIES

77STA/NUT    NBS1        .00000   10.00000       1
77STA/NUT    NBS2        .00000   10.00000       2
77STA/NUT    NBS3        .00000   10.00000       3
---          NBSPIT      .00000   10.77100       9
79PIT        PITZER      .00000    2.50000       4
77RAR/HAB    RARD        .00000    9.00000       7

END OF SEARCH

COMMAND ("M" GIVES THE MENU)?
r

WHICH REFERENCE DO YOU WANT ("A" WILL LIST ALL THIRTY-FIVE)?
77RAR/HAb

Rard, J. A., Habenschuss, A., and Spedding, F. H., J. Chem. Eng. Data *22, 180
(1977)


COMMAND ("M" GIVES THE MENU)?
q

***************EXIT FROM GAMPHI****************
```

7. Use of SUBROUTINE GAMPHI From a User-written Program

Subroutine GAMPHI is a user-callable subroutine which allows the user to specify from his own program the cation, anion, molality, and data base. The quantities which are returned are: $\gamma_{\pm}$, ϕ, the number of the equation used, the minimum and maximum molality for which data exist, the charge type of the salt, the number of parameters in the model, the parameters in the model, the literature reference, and an error indicator.

The user written program must contain the following:

```
DOUBLE PRECISION MOLAL, GAM, PHI, PARAM(150), MIN, MAX
INTEGER EQNO, CTYPE, IFAIL, NUMPAR, NIN, NOUT
CHARACTER  DBASE*8, REF*12, CATION*32, ANION*32
COMMON/BLK1/NIN, OUT
NIN = #
NOUT = #
.
.
.
CALL GAMPHI (CATION, ANION, MOLAL, DBASE, GAM,
+       PHI, MIN, MAX, CTYPE, NUMPAR, PARAM, REF, IFAIL)
```

The user must assign numerical values to the logical input and output units (NIN and NOUT).

The arguments in the SUBROUTINE are:

ANION	the name of the anion
CATION	the name of the cation
CTYPE	the charge type of the binary salt (see table 1)

DBASE	the name of the desired database (see Section 3); "P" is the recommended default.
EQNO	the number of the equation used to calculate $\gamma_{\pm}$ and ϕ
GAM	the value of the activity coefficient
IFAIL	an error indicator with the following values: 0 no errors 1 no match found for the combination of cation, anion, and database specified 2 the number of the equation used was found to be less than zero or greater than ten. This indicates that there is an error in the database used. This should not occur with the databases supplied. 3 the molality is out of range.
MAX	the maximum molality for which data exist
MIN	the minimum molality for which data exist
MOLAL	the molality at which one wishes $\gamma_{\pm}$ and ϕ to be calculated
NUMPAR	the number of parameters in the model
PARAM	the parameters in the model
PHI	the osmotic coefficient
REF	the literature reference

The first four parameters in the CALL statement must be specified in the user-written codes prior to the CALL statement; the remainder of the parameters are returned to the calling program. The cations and anions in the database are listed in Tables 2 and 3.

Table 1. Charge types of binary salts

Salt type	Charge type	ν
1-1	1	2
1-2; 2-1	2	3
1-3; 3-1	3	4
1-4; 4-1	4	5
2-2	5	2
2-3; 3-2	6	5
2-4; 4-2	7	3
3-3	8	2
3-4; 4-3	9	7
4-4	10	2
5-1; 1-5	11	6
6-1; 1-6	12	7

Table 2. Cations in the database.

H+	NH4+
Tl+	Ag+
Li+	Na+
K+	Rb+
Cs+	CN3H6+
(CH3)4N+	(ethyl)4N+
(propyl)4N+	(butyl)4N+
(CH3)3benzyl-N+	(CH3)2-O-ethylbenzyl-N+
(CH3)3S+	(HOC2H4)N+
(butyl)3S+	Mg+2
Ca+2	Sr+2
Ba+2	Fe+2
Ni+2	Co+2
Co(NH3)5NO2+2	Co(NH3)5Cl+2
Co(NH3)5F+2	Co(NH3)5CH3COO+2
Co(NH3)5CH3CH2COO+2	cis-Co(C2H8N2)NH3NO2+2
trans-Co(C2H8N2)NH3NO2+2	Co(NH3)5(CH3)2CHCOO+2
Pb+2	Cu+2
Mn+2	UO2+2
Zn+2	Cd+2
guanadinium+2	ethylenebis(trimethylammonium)+2
choline+2	Co(C2H8N2)3+3
Al+3	Sc+3
Y+3	La+3
Ce+3	Pr+3
Nd+3	Sm+3
Eu+3	Gd+3
Tb+3	Dy+3
Ho+3	Er+3
Tm+3	Yb+3
Lu+3	Ga+3
In+3	Cr+3
Th+4	

Table 3. Anions in the database.

F-	Cl-
ClO3-	ClO4-
Br-	BrO3-
I-	NO2-
NO3-	OH-
H2PO4-	H2AsO4-
PF6-	CNS-
p-toluene sulfonate-	acetate-
formate-	propionate-
butyrate-	valerate-
caproate-	heptylate-
acid-malonate-	acid-succinate-
acid-adipate-	methane sulfonate-
ethane sulfonate-	sulfonate-
benzene sulfonate-	2,5-dimethylbenzene sulfonate-
p-ethylsulfonate-	p-ethylbenzene sulfonate-
mesitylene sulfonate-	CO3-2
HPO4-2	B10H10-2
SO4-2	S2O3-2
S2O6-2	S2O8-2
HAsO4-2	B12H12-2
CrO4-2	Cr2O7-2
Pt(CN)4-2	WO4-2
1,2-ethane disulfonate-2	fumarate-2
maleate-2	2,7-anthraquinone disulfonate-2
Fe(CN)6-3	Co(CN)6-3
Mo(CN)8-4	W(CN)8-4
SO3-2	

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10. Glossary

Roman

a	activity
b	constant in Pitzer's equations
f^{γ}, f^{ϕ}	terms in Pitzer's equations
i, j	integers
m	molality
z	charge
A, A_m, A_{ϕ}	Debye-Hückel constants; $A_m = 3A_{\phi} = A\ell n(10)$
B^{γ}, B^{ϕ}	terms in Pitzer's equations
G	Gibbs energy
I	ionic strength; $I = (1/2)(\nu_c z_c^2 + \nu_a z_a^2)m$
N	number of parameters
P_1, $P_2, \ldots,$ P_i, P_j	parameters in equation
R	gas constant, 8.31441 J mol^{-1} K^{-1}
T	thermodynamic temperature
X	mole fraction

Greek

α, α_1, α_2	constants in Pitzer's equations
γ	activity coefficient
ν	ion number
ϕ	osmotic coefficient

Subscripts

$\pm$	mean ionic
a	anion
c	cation
i, j	integers
1	solvent
2	solute

Superscript

γ	see B^{γ}, f^{γ} under Roman
ϕ	see B^{ϕ}, f^{ϕ} under Roman
*	property of a pure substance.
o	standard value quantity

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☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)

A database of activity and osmotic coefficients for 350 binary aqueous electrolyte solutions at 298.15 K has been assembled together with a collection of subroutines for utilizing the database. The computer codes, which are written in FORTRAN 77, can be used either interactively or from user-written programs to calculate values of the activity and osmotic coefficients at selected molalities.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

activity coefficient; database; electrolyte solutions; FORTRAN; Gibbs energy; osmotic; salts; thermodynamics; water.

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