NATIONAL BUREAU OF STANDARDS REPORT

10 291

THERMODYNAMIC PROPERTIES OF COMPOUNDS OF BIOCHEMICAL INTEREST IN AQUEOUS SOLUTION

Eighteenth Report on
A Survey of Thermodynamic Properties of The
Compounds of The Elements CHNOPS

Technical Report
to
National Aeronautics and Space Administration
Contract No. ~~R-138~~, Amendment 4
W12-758

U.S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

NATIONAL BUREAU OF STANDARDS

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[1] Headquarters and Laboratories at Gaithersburg, Maryland, unless otherwise noted; mailing address Washington, D.C. 20234.

[2] Located at Boulder, Colorado 80302.

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R. C. Wilhoit
Jing Chao
Michael Carlo

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Contract N~~o. R-13~~8, Amendment 4

NBS

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FOREWORD

A study at the National Bureau of Standards (NBS), of which this is the eighteenth progress report, has been undertaken to meet the need of the National Aeronautics and Space Administration (NASA) for thermodynamic information on biologically related materials important to the space program for several reasons. Among these reasons are the necessity of inferring the maximum account of useful chemistry of incompletely accessible environments, for which only limited information is available, the possibility of the occurrence of organic compounds naturally synthesized under primitive conditions, and the possibility of theoretically recovering part of the prebiological history of the earth.

This program is being carried out under the technical supervision of Dr. George Jacobs of NASA, and with the consultation of Dr. Harold Morowitz of the Yale University, Department of Molecular Biology and Biophysics, and Dr. C. W. Beckett of the NBS. The contract (Contract No. R-138) was initiated 1 May 1964 and extended by Amendments 1, 2, 3, and 4. This report covers a portion of work under Amendment 4.

This report is the result of work done under NBS Contract CST-2012 for the National Bureau of Standards by a group working under the direction of Professor R. C. Wilhoit in the Thermodynamics Research Center; Texas A and M University, College Station, Texas. It covers work done in the interval May 1, 1969 to January 31, 1970, and comprises the contents of the final technical report supplied in fulfillment of that contract April 10, 1970. Tables 3-18 were revised June 12 and July 7, 1970 as noted in footnotes.

George T. Armstrong

George T. Armstrong, Chief
Thermochemistry Section

This report describes a portion of a long range project for the selection and tablulation of the thermodynamic properties of organic compounds of biological importance being conducted jointly be the Thermochemistry Section of the Division of Physical Chemistry of the National Bureau of Standards and the Thermodynamics Research Center at Texas A&M University. A method of representing the properties of binary systems, which insures thermodynamic consistency, is described and applied to the systems consisting of methanol, ethanol, n-propanol, iso-propanol, and n-butanol with water. Tables of a selected list of thermodynamic properties are presented at temperatures of 10°, 25°, and 40°C. An extensive bibliography and compound index to the thermodynamic properties of organic compounds in aqueous solution is also included.

I. Thermodynamic Properties of Binary Systems

A large amount of experimental data on the properties of binary systems derived from volumetric, calorimetric, and phase equilibria studies may be found in the published scientific literature. Such properties of any given system are not independent but are interrelated by various thermodynamic requirements. An extensive literature exists on methods of testing experimental data for thermodynamic consistency*. All of the common experimental properties can be related to the Gibbs energy of mixing of the components, and to its various derivatives with respect to concentration, temperature, and pressure. Data generated in this way are inherently thermodynamically consistent. Conversely, a variety of observed properties can be manipulated to yield information on the Gibbs energy of mixing.

These principles have been exploited to develop a procedure for generating tables of smoothed properties derived from a variety of observed data. The Gibbs energy of mixing is represented by a mathematical function of concentration and temperature involving several parameters characteristic of a particular pair of components which define a binary system. The parameters are adjusted by a least squares procedure to best represent the original data.

The calculations are based on the excess Gibbs energy of mixing, rather than the total Gibbs energy of mixing.‡

$$G^E = \frac{\Delta Gm^r - \Delta Gm^i}{(n_1 + n_2)} = \frac{\Delta Gm^r - RT(n_1 \ln X_1 + n_2 \ln X_2)}{(n_1 + n_2)} \quad (1)$$

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*see G. N. Lewis and M. Randall, "Thermodynamics", revised by K. S. Pitzer and L. Brewer, Mc-Graw-Hill Book Co., New York, 1961; E. Hala, J. Pick, V. Fried and O. Vilim, "Vapor-Liquid Equilibrium", Pergamon Press, New York, 1958; and H. C. Van Ness, "Classical Thermodynamics of Non-Electrolyte Solutions", Pergamon Press, New York, 1964 for discussions of thermodynamic principles of this problem

‡ A Glossary of mathematical symbols is given on page 8

The following equation was selected to represent the excess Gibbs energy

$$G^E = X_1 X_2 \theta_1 = X_1 X_2 (A + BX_2 + CX_2^2 + DX_2^3) \tag{2}$$

This may be transformed to the equivalent form

$$G^E = X_1 X_2 [(8A + 4B + 2C + D) + (4B + 4C + 3D)(X_2 - X_1) + (2C + 3D)(X_2 - X_1)^2 + D(X_2 - X_1)^3]/8 \tag{3}$$

The parameters A, B, C, and D are taken as functions of temperature according to

$$\begin{aligned} A &= a_1 + a_2 T + a_3 T \ln T + a_4 T^2 \\ B &= b_1 + b_2 T + b_3 T \ln T + b_4 T^2 \\ C &= c_1 + c_2 T + c_3 T \ln T + c_4 T^2 \\ D &= d_1 + d_2 T + d_3 T \ln T + d_4 T^2 \end{aligned} \tag{4}$$

This choice of function makes the excess enthalpy of mixing a quadratic function of temperature and the excess heat capacity a linear function of temperature.

$$H^E = X_1 X_2 \theta_4 = G^E - T\left(\frac{\partial G^E}{\partial T}\right)_{P, X_1, X_2} = X_1 X_2 (A' + B'X_2 + C'X_2^2 + D'X_2^3) \tag{5}$$

$$C_p^E = X_1 X_2 \theta_5 / T = -T\left(\frac{\partial^2 G^E}{\partial T^2}\right)_{P, X_1 X_2} = X_1 X_2 (A'' + B''X_2 + C''X_2^2 + D''X_2^3) \tag{6}$$

where

$$A' = a_1 - a_3 T - a_4 T^2 \tag{7}$$

and

$$A'' = - a_3 - 2a_4 T \tag{8}$$

with similar expressions for B', C', D', B'', C'', and D''. In the following equations subscript 1 indicates the solvent (water) and subscript 2 the solute (alcohol). The heat of solution of one mole of solute is therefore given by

$$\Delta Hs = H^E/X_2 = X_1 \theta_4 \tag{9}$$

and the heat of solution in an infinite amount of solvent (standard state in solution) is

$$\Delta Hs^\circ = - L_2^{\oplus} = A' \tag{10}$$

Equations for the following properties can be derived from G^E and its derivatives.

$$RT\ln\lambda_1 = X_2^{2}\theta_2 = G^{E} + X_2\left(\frac{\partial G^{E}}{\partial X_2}\right)_T = X_2^{2}[A - B + 2(B - C)X_2 + 3(C - D)X_2^{2} + 4DX_2^{3}] \qquad (11)$$

$$RT\ln\lambda_2 = X_1^{2}\theta_3 = G^{E} + X_1\left(\frac{\partial G^{E}}{\partial X_1}\right)_T = X_1^{2}[A + 2BX_2 + 3CX_2^{2} + 4DX_2^{3}] \qquad (12)$$

$$RT\ln\gamma_2 = RT\ln\lambda_2 + RT\ln X_1 - A$$

λ_1 and λ_2 are the activity coefficients of the solvent and solute respectively, which are related to the corresponding activities by

$$\lambda_1 = a_1/X_1 \qquad \text{and} \qquad \lambda_2 = a_2/X_2 \qquad (\text{[illegible]})$$

where the standard states are the pure components. Equations (11) and (12) are the Margules equations of fourth order. γ_2 is the activity coefficient of the solute,

$$\gamma_2 = a_2/m \qquad (\text{[illegible]})$$

in which the standard state is the hypothetical ideal solution at unit molality. In aqueous solutions the molality, m, is related to the mole fraction of the solute by

$$m = 55.56\,X_2/(1 - X_2)$$

To the extent that the virial equation with two terms adequately represents the P-V-T behaviour of the gaseous phase, the partial pressure of the solvent and solute in equilibrium with the liquid phase are given by

$$P_1 = Y_1P_t = X_1\lambda_1P_1^{*}\exp[(P_1^{*} - P_t)\beta_1] \qquad (\text{[illegible]})$$

$$P_2 = Y_2P_t = X_2\lambda_2P_2\exp[(P_2^{*} - P_t)\beta_2] \qquad (\text{[illegible]})$$

where β_1 and β_2 are the corresponding second virial coefficients. The freezing point depression, $\delta = T_0 - T$, is related to the activity of the solvent by

$$RT\ln a_1 = -\frac{(\overline{L}_1 + \Delta Hm)}{RT_0T}\,\delta + \frac{(\overline{C}_1 - C_1 + \Delta Cm)}{RT_0T}\,\delta^{2} \qquad (18)$$

ΔHm is the heat of fusion of the solvent and ΔCm the change in heat capacity the the solvent on melting. The osmotic coefficient is closely related to the activity of the solvent.

$$\Phi = -\frac{1000}{M_1\,m}\ln a_1 \qquad (\text{[illegible]})$$

The various types of enthalpy functions for binary solutions are

$$\Phi L_2 = H^{E}/X_2 + L_2^{*} = X_1\theta_4 + L_2^{*} \qquad (\text{[illegible]})$$

$$\Phi L_1 = H^{E}/X_1 = X_2\theta_{\text{[illegible]}} \qquad (\text{[illegible]})$$

$$\overline{L}_1 = H^E + \left(\frac{\partial H^E}{\partial X_1}\right)_T X_2 = X_2^2\left(\theta_4 - X_2 \frac{d\theta_4}{dX_2}\right) = X^{\ 2}[A' - B' + 2(B' - C')X_2 + 3(C' - D')X_2^{\ 2} + 4D'X_2^{\ 3}] \tag{22}$$

$$\overline{L_2} = H^E + \left(\frac{\partial H^E}{\partial X_2}\right)_T X_1 + L_2^\oplus = X_1^{\ 2}\left(\theta_4 - \frac{d\theta_4}{dX_2}\right) - A' = X_1^{\ 2}(A' + 2B'X_2 + 3C'X_2^{\ 2} + 4D'X_2^{\ 3}) - A' \tag{23}$$

The heat capacity functions are

$$\Phi C_1 = C_1^\oplus + C_p^E/X_1 = C_1^\oplus + X_2\theta_5 / T \tag{24}$$

$$\Phi C_2 = C_2^\oplus + C_p^E/X_2 = C_2^\oplus + X_1\theta_5 / T \tag{25}$$

$$\overline{C_1} = C_1^\oplus + C_p^E + X_1\left(\frac{\partial C_p^E}{\partial X_1}\right)_T = C_1^\oplus + \frac{X_2^2}{T}\left(\theta_5 - X_1 \frac{d\theta_5}{dX_2}\right) \tag{26}$$

$$= C_1^\oplus + X_2^2\ [A'' - B'' + 2(B'' - C'')X_2 + 3(C''- D'')X_2^2 + 4D''X_2^3]$$

$$\overline{C_2} = C_2^\oplus + C_p^E + X_2\left(\frac{\partial C_p^E}{\partial X_2}\right)_T = C_2^\oplus + \frac{X_1^2}{T}\left(\theta_5 + X_2 \frac{d\theta_5}{dX_2}\right) \tag{27}$$

$$= C_2^\oplus + X_2^2\,[A'' + 2B''X_2 \quad 3C''X_2^2 + 4D''X_2^3]$$

The heat capacity of one mole of solution is

$$C_p = X_1\overline{C_1} + X_2\overline{C_2} = X_1 C_1^\oplus + X_2 C_2^\oplus + C_p^E \tag{28}$$

Thus each of the five functions θ_j ($j = 1$-5), which are defined in equations (2), (5), (6), (11), and (12), can be calculated from the observed properties of the systems. They can also be represented mathematically in terms of the 16 parameters in equation (4). These can all be put in the compact form

$$\theta_j = \sum_{i=1}^{16} p_i u_{ij}(X_2, T) \tag{29}$$

where the p_i are the 16 parameters, $a_1, a_2, a_3, a_4, b_1, b_2, \ldots d_4$, and the $u_{ij}(X_2, T)$ are the appropriate functions of mole fraction and temperature. The 16 parameters are evaluated so as to obtain the "best" fit between calculated and observed properties by the least squares criterion. Let θ_{jk} be the value of the function θ_j calculated from the k-th experimental measurement and $u_{ijk}(X_2, T)$ be the corresponding value of the function u_{ij} at this point. The parameters, p_i, are adjusted so as to minimize the sum

$$S = \sum_{k=1}^{n} \sum_{j=1}^{5} W_k \left[\sum_{i=1}^{16} p_i u_{ijk}(X_2, T) - \theta_{jk}\right]^2 \tag{30}$$

Since the paramters appear in equations (29) and (30) as linear functions this calculation can be carried out with the usual linear least squares procedure.

The five functions θ_j are treated as a single dependent variable and the functions u_{ij} are the 16 independent variables.

The W_k in equation (30) are weighting factors associated with each observed data point. They are taken to be proportional to the reciprocals of the uncertainties in the corresponding values of θ_{jk}. These are calculated from estimates of the uncertainties of the original observed data, taking into account the mathematical relation between the properties and the θ_{jk}.

Although this procedure insures thermodynamic consistency the thermodynamic properties calculated from the 16 parameters be realistic only if the original data are adequate and if the function in equation (2) is sufficiently flexible to follow the properties of the real system. The Gibbs energy of mixing is seldom, if ever, measured directly. The properties commonly observed are related to various derivatives of G^E. For example, activity coefficients and other properties obtained from phase equilibria involve the derivative of G^E with respect to concentration. Calorimetric measurements of enthalpy changes at constant temperature are related to the derivative of G^E with respect to temperature, and heat capacity measurements are related to the second derivative with respect to temperature. Thus the original data must not only be accurate but must also be well distributed over a wide range of temperature and concentration. As a minimum it is necessary to have either phase equilibrium data and enthalpy data at closely spaced intervals over a range of concentration for at least one temperature or phase equilibrium data at several temperatures. In practice it is very difficult to obtain reliable enthalpy and heat capacity properties from phase equilibrium data alone. It is best to have all three types of properties at various temperatures and concentrations. However the usual situation is that the bulk of the phase equilibrium data are concentrated along the normal boiling and freezing point lines, while most of the enthalpy and heat capacity data are obtained in the vicinity of room temperature.

Equations (2) and (4) were chosen to represent the excess Gibbs energy of mixing because of the relative mathematical simplicity of the derivatives with respect to temperature and concentration, and also because of their convenience in carrying out least squares calculations. Many other equations which have the proper characteristics have been suggested in the literature. Aqueous solutions, especially those contiaing alcohols, acids, and ketones, demonstrate very complex behaviour. It was found, in fact, that this equation was not adequate for alcohols above ethanol, and may not be adequate even for ethanol. Although equation (2) can be made more flexible by expanding it to higher powers of X_2, it appears that 16 parameters is about the highest practical limit. Increasing the number of parameters imposes more rigorous requirements on the accuracy and distribution of the data and increases the possibility of spurious results in regions not covered by the data. More parameters also increase the effect of truncation errors in the calculation, and this can be a significant problem even in double precision mode.

For those cases in which a single set of parameters is not adequate equations (2) and (4) can still be taken as the basis for calculating thermodynamic properties by separating the data into limitted regions of temperature and composition. Sets of parameters can then be calculated independently for each region. However unless additional provisions are made the values of G^E and its derivatives calculated from different sets of apramenters will not be the same at the boundary between two regions. This will give discontinuities in the thermodynamic properties at these boundaries. Although methods of forcing the equalitiy of the dependent variable and its derivatives at such boundaries have been described for least squares calculations these would be difficult to apply here, and have not, as yet, been attempted. Theoretically the amount of such discontinuities can be reduced by carrying out a series of calculations for neighboring regions in which data calculated from one set of parameters is used as input for calculating the other set of parameters. This can be repeated until the discontinutity is reduced to the point where it is no longer significant.

The parameters in equations (2) and (4) were calculated in this manner for the binary systems consiting of the five alcohols from methanol to n-butanol and water. The calculations were carried out on an IBM 360/65 computer. Double precision arithmetic, equivalent to about 15 decimal digits, was used on the critical parts of the calculation. Additional programs were written to compare the calculated and observed properties and to generate tables of thermodynamic properties at regular intervals of temperature and pressure. Table 1 identifies the sources of data used in the final calculations. These were obtained by searching the published literature and selecting what appeared to be the best values. A series of preliminary least squares calculations were then made and the calculated properties were compared to the original ones. Additional screening was then carried out to remove large discrepancies in the data. Ranges of temperature and concentration covered by the final set of data are shown schematically in Figures 1 and 2. For this purpose the data is grouped into three main types: activity and phase equilibrium data, enthalpy data includeing heats of solution and dilution, and heat capacity data. Equation (2) does not generate reliable thermodynamic properties outside the regions of temperature and concentration covered by the original data.

Tables 2 and 3 summarize the results of the least squares calculations. Table 2 gives the following information for each kind of property entered into the calculations: number of values, average absolute value, and root mean square deviation (R. M. S. deviation). The root means square deviation of any property, z, is defined as

$$\text{R. M. S deviation} = \left(\frac{\sum_{k=1}^{n} (z_k - z_c)^2}{n} \right)^{\frac{1}{2}} \qquad (31)$$

where n is the number of data points, z_k, the k-th observed value of the property and z_c the calculated value. Comparison of the R. M. S. deviation with the average absolute value gives some indication of how well the calculated values agree with the observed data.

Values of several properties calculated at selected molalities and at temperatures of 10°, 25°, and 40°C are reported in Tables 4-18. These properties were calculated from the parameters in Table 3 for the corresponding concentration range. Since the dilute region is of more importance for biochemical applications it is given in greater detail than the concentrated region. Table 19 gives certain auxiliary data for the pure alcohols which were used in the calculations.

On the basis of intermolecular interactions water is more similar to methanol than it is to any of the other alcohols. Thus the properties of the water-methanol system are simpler and more regular than they are for the other systems. As the number of carbon atoms in the alcohol molecule increases the solubility in water decreases. While methanol, ethanol, and the two propanols are all completely miscible with water n-butanol and the higher alcohols are only partially miscible. The rapid change in the slope of the thermodynamic properties with respect to concentration for n-propanol and iso-propanol in the range of 0.1 to 0.2 mole fraction reflects the close approach to the formation of two phases in these systems. Because of its simpler behaviour and because of the large amount of accurate experimental data available the agreement between observed and calculated values is better for methanol-water than for any of the other systems. Data for the ethanol-water system are also quite extensive, and, except for the heats of solution at low concentration, the agreement between observed and calculated values is fairly good. It is probable that it would be necessary to separate the water-ethanol data into two concentration regions to obtain a better fit. Properties for the systems of the two propanols with water cannot be represented, even, approximately, by a single set of parameters. Therefore separate sets of parameters were calculated for low and high concentration regions for these systems. The boundaries occurr at 9.8 molal for n-propanol and 14 molal for iso-propanol. Values of G^E and H^E calculated from the low concentration parameters were used as input data in calculating the high concetration parameters. However, as can be seen in Tables 10-15 there are still some distinct discontinuities at the boundaries. These are especially large for enthalpy and heat capacity. This reflects the fact that there are not many good calorimetric measurements for the high concentrations, and, since these properties involve the first and second derivatives of phase equilibrium data with respect to temperature, small errors in phase equilibrium data cause large uncertainties in enthalpy and heat capacity.

The n-butanol -water system separates into two phases, identified as the water-rich, and the alcohol-rich phases. The compositions of the two phases at equilibrium depend on the temperature but are approximately 1.4 molal and 42 molal respectively. Thermodynamics requires that the activity of each component be equal in the two phases at equilibrium. Thus activities of water and alcohol calculated from the parameters for the water-rich phase were entered as data in calculating the parameters for the alcohol-rich phase. Since only phase equilibrium data were available for the alcohol-rich phase, and these were mostly confined to the temperatures of 25-30° and along the normal boiling point curve the values of enthalpy and heat capacity calculated for the alcohol-rich phase are not reliable.

Glossary of Terms and Symbols

A, A', A''	Parameters defined by equations (2), (7), and (8)
a_1, a_2, a_3, a_4	Parameters in equation (4)
a_1	Relative activity of the solvent, standard state the pure solvent
a_2	Relative activity of the solute, standard state the pure solute
a_2^*	Relative activity of the solute, standard state the hypothetical ideal solution at unit molality
B, B', B''	Parameters defined by equations (2), (7), and (8)
b_1, b_2, b_3, b_4	Parameters in equation (4)
C, C', C''	Parameters defined by equations (2), (7), and (8)
c_1, c_2, c_3, c_4	Parameters in equation (4)
C_p^E	excess heat capacity, cal $\deg^{-1}$ mol^{-1}
C_p	heat capacity of the mixture, cal $\deg^{-1}$ mol^{-1}
$\overline{C_1}$	partial molal heat capacity of the solvent in solution, cal $\deg^{-1}$mol^{-1}
$C_1^{\oplus}$	heat capacity of the pure solvent, cal $\deg^{-1}$ mol^{-1}
$\overline{C_2}$	partial molal heat capacity of the solute in solution, cal $\deg^{-1}$ mol^{-1}
$C_2^{\oplus}$	heat capacity of the pure solute, cal $\deg^{-1}$mol^{-1}
D, D', D''	Parameters defined by equations (2), (7), and (8)
d_1, d_2, d_3, d_4	Parameters in equation (4)
G^E	excess Gibbs energy of mixing, cal mol^{-1} of solution
ΔG_m^r	Gibbs energy of mixing of real solution, cal mol^{-1} of solution
ΔG_m^i	Gibbs energy of mixing of ideal solution, cal mol^{-1} of solution
ΔG_s	Gibbs energy of solution, cal mol^{-1} of solute
H^E	excess enthalpy of mixing
ΔH_s	enthalpy of solution, cal mol^{-1} of solute
ΔH_s°	enthalpy of solution at infinite dilution, cal mol^{-1} of solute
ΔH_d	enthalpy of dilution, cal mol^{-1} of solute
ΔH_m	heat of fusion of pure solvent, cal mol^{-1} of solvent
h	specific heat of the solution, cal $\deg^{-1}$ mol^{-1}
$\overline{L_1}$	relative partial molal enthalpy of the solvent, $\overline{H_1} - H_1^{\circ}$, standard state is the pure solvent, cal mol^{-1}
$\overline{L_2}$	relative partial molal enthalpy of the solute, $\overline{H_2} - H_2^{\circ}$, standard state is the solute at infinite dilution, cal mol^{-1}

$L_2^{\oplus}$	relative partial molal enthalpy of the pure solute, cal mol^{-1}
M_1	molecular weight of the solvent
m	molality of the solute, mol kg^{-1}
n_1	amount of solvent in units of moles
n_2	amount of solute in units of moles
P_t	total vapor pressure of the solution, mmHg
P_1	partial pressure of the solvent vapor in equilibrium with the solution,
$P_1^{\oplus}$	vapor pressure of the pure solvent, mmHg
P_2	partial pressure of the solute vapor in equilibrium with the solution
$P_2^{\oplus}$	vapor pressure of the pure solute, mmHg
R	gas constant, 1.98717 cal deg^{-1}mol^{-1}
T	temperature °K
T_o	freezing point of the pure solvent, 273.15°K
u_i	functions in equation (27)
W_k	weighting factor of k-th data point
X_1	mole fraction of the solvent in the liquid phase
X_2	mole fraction of the solute in the liquid phase
Y_1	mole fraction of the solvent in the vapor phase
Y_2	mole fraction of the solute in the vapor phase
β_1	second virial coefficient of the gaseous solvent
β_2	second virial coefficient of the gaseous solute
δ	freezing point depression of the solution, °K
λ_1	activity coefficient of the solvent, mole fraction basis
λ_2	activity coefficient of the solute, mole fraction basis
γ_2	activity coefficient of the solute, molal basis
$\theta_1, \theta_2, \theta_3, \theta_4, \theta_5$	functions defined by equations (2), (5), (6), (11), and (12)
Φ	osmotic coefficient
ΦC_1	apparent molal heat capacity of the solvent, cal deg^{-1}mol^{-1}
ΦC_2	apparent molal heat capacity of the solute, cal deg^{-1} mol^{-1}
ΦL_1	relative apparent molal enthalpy of the solvent, cal mol^{-1}
ΦL_2	relative apparent molal enthalpy of the solute, cal mol^{-1}

Table 1

Identification of Sources of Data Entered into the Least Squares Fit for the Thermodynamic Properties of Alcohol-Water Systems

(numbers refer to the citations in the bibliography)

Methanol
  activity and phase equilibrium data: 89, 131, 184, 221, 338, 426, 567, 609
  enthalpy data: 9, 18, 45, 53, 64, 338, 354, 358, 458
  heat capacity data: 64, 338

Ethanol
  activity and phase equilibrium data: 49, 124, 131, 146, 293, 338, 380, 408, 609
  enthalpy data: 9, 18, 22, 53, 64, 68, 263, 338, 351, 358
  heat capacity data: 64, 338, 484

n-Propanol, low concentration range
  activity and phase equilibrium data: 87, 89, 195, 241, 338, 417, 490, 609
  enthalpy data: 9, 18, 22, 23, 39, 64, 142, 294, 263, 338, 351
  heat capacity data: 64, 338

n-Propanol, high concentration range
  activity and phase equilibrium data: 89, 195, 241
  enthalpy data: 39, 194
  heat capacity data: 64

iso-Propanol, low concentration range
  activity and phase equilibrium data: 79, 89, 338, 569, 609, 615
  enthalpy data: 9, 18, 142, 263, 301, 338, 351, 354
  heat capacity data: 301, 338

iso-Propanol, high concentration range
  activity and phase equilibrium data: 79, 569, 615
  enthalpy data: 301. 354
  heat capacity data: 301

n-Butanol, water-rich phase
  activity and phase equilibrium data: 87, 89, 172, 260, 338, 469, 526, 535, 588
  enthalpy data: 9, 18, 23, 263, 338, 351
  heat capacity data: 338

n-Butanol, alcohol-rich phase
  activity and phase equilibrium data: 87, 172, 260, 469, 526, 535

Table 2. Thermodynamic Properties of Binary Systems of Alcohols and Water

Summary of Least Squares Fitting Computations

Solute	Methanol	Ethanol	n-Propanol	n-Propanol	iso-Propanol	iso-Propanol	n-Butanol	n-Butanol
Data Set Number	11	7	10	12	6	8	5	6
Number of data points	406	421	178	176	192	167	116	73
Range of Data								
molality	0 - ∞	0 - ∞	0 - 9.8	9.8 - ∞	0 - 14	14 - ∞	0 - 1.4	42 - ∞
temperature, °C	-10 - 100	-8 - 100	-4 - 95	0 - 95	-7 - 99	+10 - 81	-3 - 99	+25 - 115

Comparison of Calculated with Observed Data

Solute	Methanol	Ethanol	n-Propanol	n-Propanol	iso-Propanol	iso-Propanol	n-Butanol	n-Butanol
Property: activity of solute, a_2								
number of points	0	0	0	0	0	0	1	15
avg. abs. value							0.368	0.822
R. M. S. deviation							0.009	0.017
Property: activity coefficient of the solute, λ_2								
number of points	9	0	12	29	1	0	1	0
avg. abs. value	1.09		6.65	1.41	7.70		52.9	
R. M. S. deviation	0.037		0.661	0.122	1.39		2.2	
Property: logarathm of activity coefficient, $\ln\lambda_2$								
number of points	0	0	2	8	0	0	0	0
avg. abs. value			2.106	0.607				
R. M. S. deviation			0.720	0.189				
Property: vapor pressure of the solute, P_2, mm								
number of points	10	7	5	6	16	30	2	2
avg. abs. value	130.1	23.4	9.07	16.8	53.0	115.2	3.92	5.68
R. M. S. deviation	1.90	1.08	0.71	1.97	6.50	5.78	0.15	0.64
Property: mole fraction of solute in the vapor phase, Y_2								
number of points	71	118	6	11	37	86	23	41
avg. abs. value	0.538	0.463	0.294	0.561	0.373	0.675	0.168	0.431
R. M. S. deviation	0.016	0.037	0.016	0.063	0.028	0.030	0.009	0.011

Table 2. (continued)

	Methanol	Ethanol	n-Propanol	n-Propanol	iso-Propanol	iso-Propanol	n-Butanol	n-Butanol
roperty: activity of the solvent, a_1								
umber of points	0	0	0	0	0	0	1	15
vg. abs. value							0.990	0.765
							0.003	0.099
roperty: activity coefficient of the solvent, λ_1								
umber of points	9	0	0	0	0	0	0	0
vg. abs. value	1.093							
R. M. S. deviation	0.037							
roperty: freezing point depression, δ °C								
umber of points	50	51	29	0	41	0	44	0
avg. abs. value	3.187	2.035	1.558		2.100		0.765	
R. M. S. deviation	0.129	0.025	0.288		0.294		0.016	
roperty: excess enthalpy of mixing, H^E, cal mol^{-1} of solution								
number of points	120	108	43	82	29	26	10	0
avg. abs. value	149.8	106.2	79.4	52.6	127.4	52.1	46.7	
R. M. S. deviation	56.8	38.8	8.47	17.9	6.8	16.4	0.76	
roperty: $H^E/(X_1X_2)$, cal mol^{-1}								
number of points	5	4	0	0	0	0	0	0
avg. abs. value	1810.4	2610.2						
R. M. S. deviation	26.7	393.1						
roperty: heat of solution, ΔH_s, cal mol^{-1} of solute								
number of points	1	6	17	0	12	0	14	0
avg. abs. value	1754.0	2406.3	2330.8		2936.0		2199.9	
R. M. S. deviation	17.9	386.4	135.6		110.9		95.8	
Property: Relative partial molal enthalpy, $\overline{L}_1$, cal mol^{-1}								
number of points	9	11	0	0	0	0	0	0
avg. abs. value	301.7	157.1						
R. M. S. deviation	63.6	61.4						

Table 2. (continued)

	Methanol	Ethanol	n-Propanol	n-Propanol	iso-Propanol	iso-Propanol	n-Butanol	n-Butanol
Property: relative apparent molal enthalpy, ΦL_2, cal mol^{-1}								
number of points	13	0	0	0	0	0	0	0
avg. abs. value	86.0							
R. M. S. deviation	11.7							
Property: heat of dilution, ΔH_d, cal mol^{-1} of solute								
number of points	13	10	10	0	14	0	0	0
avg. abs. value	12.0	10.3	26.1		562.3			
R. M. S. deviation	2.39	3.88	0.73		184.3			
Property: specific heat of the solution, h, cal deg^{-1} g^{-1}								
number of points	56	78	24	35	0	0	0	0
avg. abs. value	0.843	0.874	1.021	0.784				
R. M. S. deviation	0.011	0.021	0.032	0.135				
Property: heat capacity of the solution, C_p, cal deg^{-1} mol^{-1}								
number of points	40	28	30	0	42	25	20	0
avg. abs. value	18.9	20.2	21.1		21.9	33.8	19.5	
R. M. S. deviation	0.27	0.58	1.15		0.61	5.19	0.29	

Table 3

Numerical Values of Parameters in Equation (4) from Least Squares Calculation

	Methanol	Ethanol	Ethanol	n-Propanol	n-Propanol	iso-Propanol	iso-Propanol	n-Butanol	n-Butanol
range of molality	0 - ∞	0 - 14	14 - ∞	0 - 9.8	9.8 - ∞	0 - 14	14 - ∞	0 - 1.4	42 - ∞
$a_1 \times 10^{-4}$	-1.426567	-2.681153	-2.070652	-3.325973	-2.325295	-1.484272	-5.699351	-4.403041	-1430.150
$a_2 \times 10^{-3}$	0.4176052	0.7907417	0.5659524	0.9712568	0.6947976	0.2442485	1.914527	1.348754	481.4916
$a_3 \times 10^{-2}$	-0.6958054	-1.311920	-0.9211317	-1.598260	-1.143315	-0.3229585	-3.263401	-2.241216	-822.5050
$a_4 \times 10$	0.9243762	1.655038	1.037934	1.876236	1.340342	-0.2274581	4.713144	2.804970	1177.142
$b_1 \times 10^{-4}$	7.719469	10.66938	8.947881	-54.41441	13.87444	-42.49051	21.74846	-0.4838133	5714.614
$b_2 \times 10^{-3}$	-2.630878	-4.328703	-2.607274	18.45489	-4.635242	14.00195	-7.294363	-5.314063	-1903.342
$b_3 \times 10^{-2}$	4.513264	7.699229	4.337329	-31.48880	7.909143	-23.72127	12.45070	11.46905	3243.711
$b_4 \times 10$	-6.681843	-13.96788	-5.473378	43.93384	-11.49799	31.63783	-17.91006	-39.94453	-4574.678
$c_1 \times 10^{-4}$	-12.63566	-0.9577277	-12.63447	1028.317	-25.30840	170.5421	-33.64971	7487.429	-6461.206
$c_2 \times 10^{-3}$	4.570578	11.24613	3.797507	-339.0889	8.683906	-25.00656	11.17430	-2587.888	2113.520
$c_3 \times 10^{-2}$	-7.915154	-23.33056	-6.373694	576.1530	-14.90952	30.30118	-19.00695	4438.648	-3587.365
$c_4 \times 10$	12.17517	69.93882	8.488408	-794.4296	22.34831	67.19030	26.50370	-6468.076	4931.160
$d_1 \times 10^{-4}$	6.341995	-16.82243	5.803186	-3671.861	15.45912	137.4587	17.48412	0.000000	1572.777
$d_2 \times 10^{-3}$	-2.396337	-25.08110	-1.781041	1202.870	-5.377262	-173.4256	-5.729617	0.000000	-494.8280
$d_3 \times 10^{-2}$	4.173638	54.34871	3.004988	-2041.646	9.258728	344.1377	9.705559	0.000000	832.3319
$d_4 \times 10$	-6.541940	-179.2110	-4.121087	2802.490	-14.06200	-914.7098	-13.09524	0.000000	-1077.016

TABLE 4

THERMODYNAMIC PROPERTIES OF THE SYSTEM METHANOL–WATER AT 10°C

Molality m	Activity of solvent a_1	Act.Coeff. of solute γ_2	Gibbs Energy of solution ΔG_S cal mol-1	Heat of solution ΔH_S cal mol-1	Partial Molal Enthalpy		Partial Molal Heat Capacity	
					solvent, $\overline{L}_1$ cal mol-1	solute, $\overline{L}_2$ cal mol-1	solvent, $\overline{C}_1$ cal deg-1 mol-1	solute, $\overline{C}_2$
0.00	1.0000	1.0000	-2105.1*	-1975.0*	0.0	0.0	18.06	35.98
0.02	0.9996	0.9997	-4867.8	-1973.2	-0.0	3.6	18.06	35.92
0.05	0.9991	0.9993	-4353.3	-1970.6	-0.0	8.9	18.06	35.82
0.10	0.9982	0.9985	-3963.8	-1966.1	-0.0	17.8	18.06	35.66
0.15	0.9973	0.9978	-3735.7	-1961.7	-0.0	26.6	18.06	35.50
0.20	0.9964	0.9971	-3574.2	-1957.3	-0.1	35.4	18.06	35.34
0.30	0.9946	0.9956	-3346.4	-1948.5	-0.1	52.8	18.07	35.03
0.40	0.9928	0.9941	-3185.0	-1939.8	-0.3	70.1	18.07	34.72
0.50	0.9911	0.9926	-3059.8	-1931.1	-0.4	87.3	18.07	34.42
0.60	0.9893	0.9912	-2957.7	-1922.4	-0.6	104.3	18.07	34.12
0.70	0.9875	0.9897	-2871.4	-1913.9	-0.8	121.1	18.08	33.83
0.80	0.9858	0.9882	-2796.6	-1905.3	-1.0	137.9	18.08	33.54
0.90	0.9840	0.9867	-2730.8	-1896.8	-1.2	154.5	18.08	33.26
1.00	0.9823	0.9853	-2671.9	-1888.4	-1.5	170.9	18.09	32.98
1.20	0.9788	0.9823	-2570.2	-1871.6	-2.2	203.4	18.10	32.43
1.40	0.9754	0.9793	-2484.3	-1855.1	-2.9	235.3	18.11	31.91
1.60	0.9719	0.9763	-2410.0	-1838.7	-3.8	266.6	18.13	31.39
1.80	0.9685	0.9733	-2344.6	-1822.5	-4.7	297.5	18.14	30.90
2.00	0.9651	0.9703	-2286.2	-1806.5	-5.7	327.8	18.16	30.42
2.50	0.9568	0.9628	-2162.8	-1767.2	-8.7	401.3	18.20	29.28
3.00	0.9486	0.9553	-2062.3	-1729.1	-12.2	471.7	18.26	28.23
4.00	0.9326	0.9401	-1904.9	-1655.9	-20.5	603.6	18.37	26.37
5.00	0.9171	0.9249	-1783.7	-1586.7	-30.3	724.5	18.50	24.78
6.00	0.9023	0.9096	-1685.7	-1521.3	-41.3	835.3	18.64	23.43
7.00	0.8879	0.8943	-1603.5	-1459.5	-53.1	936.8	18.77	22.28
8.00	0.8741	0.8791	-1533.0	-1400.9	-65.7	1029.7	18.90	21.30
9.00	0.8608	0.8640	-1471.4	-1345.5	-7[illegible].7	1114.7	19.03	20.48
10.00	0.8479	0.8489	-1416.9	-1293.0	-92.0	1192.4	19.15	19.78
12.00	0.8237	0.8194	-1323.8	-1196.3	-118.9	1328.7	19.36	18.70
14.00	0.8012	0.7907	-1246.8	-1109.3	-145.5	1442.5	19.53	17.95
16.00	0.7804	0.7629	-1181.5	-1031.1	-171.1	1537.6	19.67	17.44
18.00	0.7610	0.7362	-1125.0	-960.6	-195.4	1616.9	19.77	17.10
20.00	0.7430	0.7106	-1075.6	-897.0	-217.9	1682.9	19.84	16.91
30.00	0.6694	0.6002	-896.5	-657.9	-302.5	1876.8	19.82	16.91
40.00	0.6150	0.5157	-781.7	-507.7	-345.1	1946.2	19.50	17.42
50.00	0.5724	0.4510	-700.4	-409.6	-359.0	1963.9	19.12	17.89
60.00	0.5373	0.4007	-639.2	-343.3	-356.0	1961.0	18.78	18.23
80.00	0.4808	0.3286	-551.7	-263.5	-329.1	1939.9	18.31	18.62
100.00	0.4353	0.2796	-490.8	-219.8	-299.0	1921.2	18.07	18.77
150.00	0.3493	0.2059	-394.1	-168.5	-260.5	1902.9	17.98	18.82
200.00	0.2883	0.1642	-334.7	-144.3	-268.9	1905.4	18.09	18.78
INF	0.0000	0.0000	0.0	0.0	-1161.8	1975.0	17.50	18.75

* STANDARD STATE VALUES
JUNE 12,1970

TABLE 5

THERMODYNAMIC PROPERTIES OF THE SYSTEM METHANOL–WATER AT 25°C

Molality m	Activity of solvent a_1	Act.Coeff. of solute γ_2	Gibbs Energy of solution ΔG_S cal mol^{-1}	Heat of solution ΔH_S cal mol^{-1}	Partial Molal Enthalpy solvent, $\overline{L}_1$ cal mol^{-1}	solute, $\overline{L}_2$ cal mol^{-1}	Partial Molal Heat Capacity solvent, $\overline{C}_1$ cal deg^{-1}	solute, $\overline{C}_2$ mol^{-1}
0.00	1.0000	1.0000	-2118.4*	-1737.3*	0.0	0.0	18.00	33.85
0.02	0.9996	0.9994	-5027.5	-1736.0	-0.0	2.7	18.00	33.80
0.05	0.9991	0.9986	-4485.9	-1733.9	-0.0	6.8	18.00	33.73
0.10	0.9982	0.9971	-4075.9	-1730.6	-0.0	13.5	18.00	33.61
0.15	0.9973	0.9957	-3836.0	-1727.2	-0.0	20.3	18.00	33.49
0.20	0.9964	0.9943	-3666.1	-1723.8	-0.0	27.0	18.00	33.37
0.30	0.9946	0.9915	-3426.7	-1717.1	-0.1	40.3	18.00	33.14
0.40	0.9929	0.9887	-3257.1	-1710.4	-0.2	53.6	18.00	32.91
0.50	0.9911	0.9859	-3125.7	-1703.8	-0.3	66.8	18.00	32.68
0.60	0.9893	0.9831	-3018.6	-1697.1	-0.4	79.9	18.01	32.46
0.70	0.9876	0.9803	-2928.1	-1690.5	-0.6	92.9	18.01	32.24
0.80	0.9859	0.9776	-2849.8	-1684.0	-0.8	105.8	18.01	32.02
0.90	0.9841	0.9748	-2780.9	-1677.4	-1.0	118.7	18.01	31.81
1.00	0.9824	0.9721	-2719.3	-1670.9	-1.2	131.5	18.02	31.60
1.20	0.9790	0.9667	-2612.9	-1657.9	-1.7	156.7	18.03	31.18
1.40	0.9756	0.9613	-2523.3	-1645.1	-2.3	181.7	18.04	30.78
1.60	0.9722	0.9560	-2445.8	-1632.4	-2.9	206.3	18.05	30.39
1.80	0.9689	0.9507	-2377.7	-1619.8	-3.7	230.6	18.06	30.02
2.00	0.9656	0.9455	-2316.9	-1607.3	-4.5	254.5	18.07	29.65
2.50	0.9574	0.9327	-2188.8	-1576.5	-6.9	313.0	18.10	28.78
3.00	0.9495	0.9202	-2084.9	-1546.4	-9.6	369.5	18.14	27.98
4.00	0.9341	0.8960	-1922.5	-1488.2	-16.4	476.6	18.24	26.53
5.00	0.9194	0.8728	-1798.3	-1432.6	-24.5	576.2	18.34	25.28
6.00	0.9053	0.8506	-1698.1	-1379.6	-33.6	668.8	18.44	24.20
7.00	0.8917	0.8294	-1614.6	-1328.9	-43.7	754.7	18.55	23.27
8.00	0.8788	0.8090	-1543.2	-1280.6	-54.4	834.2	18.66	22.47
9.00	0.8663	0.7895	-1481.0	-1234.5	-65.7	907.9	18.77	21.78
10.00	0.8544	0.7707	-1426.1	-1190.6	-77.3	976.0	18.87	21.19
12.00	0.8318	0.7354	-1332.9	-1108.7	-101.2	1097.0	19.05	20.24
14.00	0.8109	0.7028	-1256.0	-1034.2	-125.3	1200.0	19.22	19.54
16.00	0.7916	0.6726	-1191.1	-966.5	-148.9	1287.4	19.35	19.03
18.00	0.7736	0.6446	-1135.2	-904.9	-171.5	1361.5	19.46	18.67
20.00	0.7567	0.6187	-1086.3	-848.8	-192.9	1424.0	19.55	18.42
30.00	0.6869	0.5136	-909.7	-633.7	-276.6	1615.3	19.70	18.05
40.00	0.6336	0.4385	-796.5	-494.9	-322.5	1690.0	19.57	18.25
50.00	0.5906	0.3828	-716.0	-402.5	-340.9	1713.2	19.35	18.52
60.00	0.5544	0.3401	-654.9	-339.2	-342.2	1714.7	19.12	18.76
80.00	0.4950	0.2793	-566.9	-261.8	-321.7	1698.7	18.74	19.07
100.00	0.4471	0.2380	-505.2	-218.9	-295.4	1682.4	18.48	19.23
150.00	0.3576	0.1756	-406.0	-167.9	-259.6	1665.5	18.20	19.36
200.00	0.2954	0.1400	-344.7	-143.8	-267.7	1667.8	18.13	19.38
INF	0.0000	0.0000	0.0	0.0	-1167.4	1737.3	17.81	19.39

* STANDARD STATE VALUES

JUNE 12,1970

TABLE 6

THERMODYNAMIC PROPERTIES OF THE SYSTEM METHANOL–WATER AT 40°C

Molality m	Activity of solvent a_1	Act. Coeff. of solute γ_2	Gibbs Energy of solution ΔG_S cal mol^{-1}	Heat of solution ΔH_S cal mol^{-1}	Partial Molal Enthalpy solvent, $\overline{L}_1$ cal mol^{-1}	Partial Molal Enthalpy solute, $\overline{L}_2$ cal mol^{-1}	Partial Molal Heat Capacity solvent, $\overline{C}_1$ cal deg^{-1} mol^{-1}	Partial Molal Heat Capacity solute, $\overline{C}_2$ cal deg^{-1} mol^{-1}
0.00	1.0000	1.0000	-2142.6*	-1541.2*	0.0	0.0	17.98	31.66
0.02	0.9996	0.9992	-5198.1	-1540.2	-0.0	2.1	17.98	31.62
0.05	0.9991	0.9981	-4629.3	-1538.6	-0.0	5.3	17.98	31.58
0.10	0.9982	0.9962	-4198.9	-1536.0	-0.0	10.5	17.98	31.50
0.15	0.9973	0.9943	-3947.0	-1533.3	-0.0	15.8	17.98	31.42
0.20	0.9964	0.9924	-3768.7	-1530.7	-0.0	21.0	17.98	31.34
0.30	0.9946	0.9886	-3517.6	-1525.5	-0.1	31.4	17.98	31.18
0.40	0.9929	0.9849	-3339.8	-1520.2	-0.2	41.8	17.98	31.03
0.50	0.9911	0.9812	-3202.1	-1515.0	-0.2	52.2	17.99	30.88
0.60	0.9894	0.9775	-3089.8	-1509.8	-0.3	62.5	17.99	30.73
0.70	0.9876	0.9738	-2995.1	-1504.7	-0.5	72.8	17.99	30.58
0.80	0.9859	0.9702	-2913.1	-1499.5	-0.6	83.0	17.99	30.44
0.90	0.9842	0.9665	-2841.1	-1494.4	-0.8	93.1	17.99	30.29
1.00	0.9825	0.9630	-2776.7	-1489.2	-0.9	103.3	18.00	30.15
1.20	0.9791	0.9558	-2665.5	-1479.0	-1.3	123.3	18.00	29.87
1.40	0.9757	0.9488	-2571.9	-1468.9	-1.8	143.3	18.01	29.60
1.60	0.9724	0.9419	-2491.1	-1458.8	-2.3	163.0	18.01	29.34
1.80	0.9691	0.9351	-2420.2	-1448.7	-2.9	182.5	18.02	29.08
2.00	0.9659	0.9283	-2356.9	-1438.8	-3.6	201.8	18.03	28.83
2.50	0.9579	0.9118	-2223.7	-1414.1	-5.5	249.2	18.06	28.22
3.00	0.9502	0.8959	-2115.9	-1389.9	-7.8	295.4	18.08	27.66
4.00	0.9352	0.8654	-1948.0	-1342.7	-13.4	384.0	18.15	26.63
5.00	0.9210	0.8369	-1820.1	-1297.2	-20.1	467.5	18.22	25.72
6.00	0.9075	0.8100	-1717.3	-1253.3	-27.9	545.9	18.30	24.92
7.00	0.8946	0.7847	-1631.9	-1211.2	-36.5	619.5	18.38	24.21
8.00	0.8823	0.7609	-1559.2	-1170.6	-45.8	688.4	18.47	23.58
9.00	0.8706	0.7384	-1496.0	-1131.7	-55.6	752.6	18.55	23.03
10.00	0.8593	0.7171	-1440.4	-1094.4	-65.9	812.6	18.64	22.54
12.00	0.8382	0.6779	-1346.3	-1024.2	-87.2	920.3	18.80	21.72
14.00	0.8187	0.6427	-1269.1	-959.8	-108.9	1013.3	18.95	21.08
16.00	0.8006	0.6110	-1204.0	-900.7	-130.5	1093.1	19.08	20.57
18.00	0.7837	0.5822	-1148.2	-846.5	-151.4	1161.5	19.21	20.18
20.00	0.7680	0.5560	-1099.5	-796.8	-171.3	1219.9	19.31	19.87
30.00	0.7018	0.4547	-924.3	-603.6	-251.5	1402.9	19.63	19.14
40.00	0.6498	0.3858	-812.1	-476.4	-297.9	1478.2	19.70	19.02
50.00	0.6066	0.3361	-732.1	-390.6	-318.4	1504.0	19.63	19.09
60.00	0.5695	0.2986	-671.1	-331.2	-322.3	1508.2	19.51	19.22
80.00	0.5078	0.2455	-582.4	-257.9	-307.0	1496.3	19.21	19.45
100.00	0.4577	0.2094	-519.7	-216.7	-284.5	1482.4	18.94	19.62
150.00	0.3651	0.1547	-418.0	-167.2	-254.4	1468.1	18.48	19.84
200.00	0.3018	0.1233	-354.9	-143.5	-264.9	1471.3	18.23	19.92
INF	0.0000	0.0000	0.0	0.0	-1167.3	1541.2	18.17	19.97

* STANDARD STATE VALUES
JUNE 12,1970

TABLE 7

THERMODYNAMIC PROPERTIES OF THE SYSTEM ETHANOL–WATER AT 10°C

Molality m	Activity of solvent a_1	Act.Coeff. of solute γ_2	Gibbs Energy of solution ΔG_S cal mol^{-1}	Heat of solution ΔH_S cal mol^{-1}	Partial Molal Enthalpy		Partial Molal Heat Capacity	
					solvent, $\bar{L}_1$ cal mol^{-1}	solute, $\bar{L}_2$ cal mol^{-1}	solvent, $\bar{C}_1$ cal deg^{-1} mol^{-1}	solute, $\bar{C}_2$
0.00	1.0000	1.0000	-1635.1*	-2933.6*	0.0	0.0	18.06	63.11
0.02	0.9996	0.9987	-4398.1	-2932.3	-0.0	2.6	18.06	63.09
0.05	0.9991	0.9967	-3884.0	-2930.3	-0.0	6.7	18.06	63.07
0.10	0.9982	0.9936	-3495.2	-2926.8	-0.0	13.8	18.06	63.03
0.15	0.9973	0.9904	-3267.8	-2923.2	-0.0	21.3	18.06	62.98
0.20	0.9964	0.9874	-3106.9	-2919.5	-0.1	29.3	18.06	62.93
0.30	0.9947	0.9814	-2880.6	-2911.7	-0.1	46.2	18.06	62.79
0.40	0.9929	0.9758	-2720.4	-2903.3	-0.2	64.6	18.07	62.63
0.50	0.9912	0.9703	-2596.5	-2894.5	-0.4	84.5	18.07	62.44
0.60	0.9894	0.9650	-2495.5	-2885.2	-0.6	105.6	18.07	62.23
0.70	0.9877	0.9600	-2410.4	-2875.4	-0.9	128.0	18.07	61.99
0.80	0.9860	0.9551	-2336.8	-2865.3	-1.2	151.6	18.08	61.73
0.90	0.9843	0.9504	-2272.1	-2854.6	-1.6	176.3	18.08	61.44
1.00	0.9826	0.9459	-2214.3	-2843.6	-2.0	202.1	18.08	61.14
1.20	0.9793	0.9374	-2114.6	-2820.5	-3.1	256.7	18.10	60.47
1.40	0.9759	0.9294	-2030.6	-2795.8	-4.5	314.9	18.12	59.73
1.60	0.9726	0.9220	-1958.2	-2769.9	-6.1	376.3	18.14	58.92
1.80	0.9693	0.9151	-1894.5	-2742.7	-8.1	440.6	18.16	58.06
2.00	0.9661	0.9086	-1837.6	-2714.4	-10.4	507.2	18.19	57.15
2.50	0.9581	0.8939	-1717.8	-2639.5	-17.5	682.3	18.29	54.69
3.00	0.9502	0.8809	-1620.5	-2559.6	-26.6	865.4	18.43	52.04
4.00	0.9347	0.8580	-1468.2	-2390.0	-50.2	1239.5	18.78	46.49
5.00	0.9199	0.8369	-1351.2	-2214.2	-79.5	1602.2	19.22	41.00
6.00	0.9058	0.8154	-1256.6	-2038.9	-112.3	1934.0	19.72	35.92
7.00	0.8927	0.7922	-1177.9	-1869.3	-145.9	2221.3	20.24	31.50
8.00	0.8806	0.7667	-1110.9	-1709.4	-177.5	2455.6	20.72	27.92
9.00	0.8699	0.7385	-1053.1	-1562.3	-204.3	2631.5	21.13	25.28
10.00	0.8606	0.7077	-1002.9	-1430.0	-223.9	2746.6	21.41	23.62
12.00	0.8470	0.6398	-920.5	-1215.5	-232.6	2794.1	21.45	23.33
14.00	0.8352	0.5818	-856.5	-1068.1	-237.9	2808.6	20.87	25.86
16.00	0.8238	0.5357	-804.4	-943.9	-263.6	2904.1	21.18	24.72
18.00	0.8142	0.4947	-761.2	-838.3	-284.1	2971.5	21.43	23.90
20.00	0.8061	0.4586	-724.6	-748.2	-299.9	3017.8	21.62	23.34
30.00	0.7777	0.3318	-603.6	-455.0	-324.9	3079.8	21.92	22.58
40.00	0.7566	0.2601	-534.9	-308.7	-300.4	3041.7	21.61	23.06
50.00	0.7348	0.2157	-489.3	-230.3	-261.5	2993.6	21.10	23.70
60.00	0.7107	0.1859	-455.6	-185.2	-223.9	2955.5	20.57	24.24
80.00	0.6575	0.1483	-406.7	-139.6	-170.6	2912.3	19.71	24.93
100.00	0.6039	0.1251	-370.9	-117.8	-145.7	2896.6	19.16	25.27
150.00	0.4895	0.0917	-308.8	-91.5	-149.4	2897.4	18.59	25.54
200.00	0.4068	0.0730	-267.1	-76.4	-181.8	2907.7	18.47	25.58
INF	0.0000	0.0000	0.0	0.0	-339.0	2933.6	17.17	25.64

* STANDARD STATE VALUES
JUNE 12,1970,

TABLE 8

THERMODYNAMIC PROPERTIES OF THE SYSTEM ETHANOL–WATER AT 25°C

Molality m	Activity of solvent a_1	Act.Coeff. of solute γ_2	Gibbs Energy of solution ΔG_S cal mol-1	Heat of solution ΔH_S cal mol-1	Partial Molal Enthalpy solvent, $\overline{L}_1$ cal mol-1	Partial Molal Enthalpy solute, $\overline{L}_2$ cal mol-1	Partial Molal Heat Capacity solvent, $\overline{C}_1$ cal deg-1 mol-1	Partial Molal Heat Capacity solute, $\overline{C}_2$ cal deg-1 mol-1
0.00	1.0000	1.0000	-1580.3*	-2408.8*	0.0	0.0	18.00	59.40
0.02	0.9996	0.9985	-4489.7	-2407.5	-0.0	2.7	18.00	59.42
0.05	0.9991	0.9962	-3948.5	-2405.4	-0.0	6.8	18.00	59.45
0.10	0.9982	0.9923	-3539.2	-2402.0	-0.0	14.0	18.00	59.49
0.15	0.9973	0.9886	-3300.0	-2398.4	-0.0	21.3	18.00	59.53
0.20	0.9964	0.9848	-3130.8	-2394.7	-0.1	29.0	18.00	59.55
0.30	0.9947	0.9775	-2892.8	-2387.1	-0.1	45.1	18.00	59.57
0.40	0.9929	0.9703	-2724.6	-2379.1	-0.2	62.2	18.00	59.56
0.50	0.9912	0.9632	-2594.6	-2370.8	-0.4	80.3	18.00	59.51
0.60	0.9895	0.9563	-2488.8	-2362.2	-0.6	99.3	18.00	59.44
0.70	0.9878	0.9495	-2399.6	-2353.3	-0.8	119.1	18.00	59.33
0.80	0.9861	0.9428	-2322.7	-2344.1	-1.1	139.7	18.00	59.20
0.90	0.9844	0.9363	-2255.1	-2334.6	-1.4	161.1	18.00	59.04
1.00	0.9828	0.9299	-2194.7	-2324.8	-1.8	183.2	18.01	58.86
1.20	0.9795	0.9174	-2090.9	-2304.4	-2.7	229.5	18.02	58.42
1.40	0.9763	0.9053	-2003.7	-2283.1	-3.8	278.2	18.03	57.89
1.60	0.9731	0.8936	-1928.7	-2260.9	-5.2	329.1	18.04	57.29
1.80	0.9700	0.8822	-1862.9	-2237.8	-6.8	381.8	18.07	56.01
2.00	0.9669	0.8712	-1804.4	-2214.1	-8.7	436.1	18.09	55.87
2.50	0.9594	0.8451	-1681.9	-2151.8	-14.4	577.1	18.18	53.80
3.00	0.9522	0.8206	-1583.3	-2086.4	-21.6	723.0	18.29	51.47
4.00	0.9385	0.7758	-1431.0	-1949.3	-40.2	1017.6	18.61	46.43
5.00	0.9258	0.7352	-1316.1	-1809.1	-63.1	1300.7	19.02	41.31
6.00	0.9140	0.6976	-1224.9	-1670.4	-88.6	1558.5	19.50	36.54
7.00	0.9031	0.6625	-1150.0	-1536.8	-114.7	1781.8	19.98	32.40
8.00	0.8932	0.6292	-1087.1	-1411.2	-139.4	1964.5	20.42	29.11
9.00	0.8842	0.5976	-1033.2	-1295.7	-160.5	2103.0	20.78	26.77
10.00	0.8762	0.5674	-986.6	-1191.7	-176.3	2195.9	21.00	25.47
12.00	0.8629	0.5108	-910.0	-1021.9	-185.6	2245.5	20.88	26.02
14.00	0.8516	0.4634	-849.6	-902.2	-197.9	2291.1	20.53	27.64
16.00	0.8418	0.4233	-800.8	-799.0	-219.1	2369.9	20.82	26.56
18.00	0.8334	0.3888	-760.3	-711.3	-236.0	2425.3	21.05	25.78
20.00	0.8261	0.3591	-726.2	-636.5	-248.9	2463.2	21.24	25.22
30.00	0.7986	0.2585	-613.0	-393.4	-268.8	2512.8	21.62	24.32
40.00	0.7754	0.2033	-547.7	-272.6	-248.1	2480.5	21.42	24.62
50.00	0.7507	0.1693	-503.5	-207.8	-216.1	2441.0	21.02	25.12
60.00	0.7238	0.1463	-470.2	-170.5	-185.8	2410.2	20.58	25.56
80.00	0.6669	0.1171	-420.9	-132.4	-144.5	2376.7	19.84	26.16
100.00	0.6113	0.0989	-384.3	-113.7	-127.5	2365.9	19.33	26.48
150.00	0.4959	0.0725	-320.2	-89.8	-140.0	2370.8	18.73	26.76
200.00	0.4135	0.0576	-277.2	-75.5	-174.7	2381.9	18.54	26.82
INF	0.0000	0.0000	0.0	0.0	-350.8	2408.8	17.31	26.90

* STANDARD STATE VALUES
JUNE 12,1970,

TABLE 9

THERMODYNAMIC PROPERTIES OF THE SYSTEM ETHANOL–WATER AT 40°C

Molality m	Activity of solvent a_1	Act.Coeff. of solute γ_2	Gibbs Energy of solution ΔG_S cal mol^{-1}	Heat of solution ΔH_S cal mol^{-1}	Partial Molal Enthalpy		Partial Molal Heat Capacity	
					solvent, $\bar{L}_1$ cal mol^{-1}	solute, $\bar{L}_2$ cal mol^{-1}	solvent, $\bar{C}_1$ cal deg^{-1} mol^{-1}	solute, $\bar{C}_2$
0.00	1.0000	1.0000	-1550.1*	-1958.5*	0.0	0.0	17.98	55.90
0.02	0.9996	0.9982	-4605.9	-1956.9	-0.0	3.3	17.98	55.95
0.05	0.9991	0.9956	-4037.6	-1954.4	-0.0	8.2	17.98	56.03
0.10	0.9982	0.9911	-3607.9	-1950.3	-0.0	16.6	17.98	56.15
0.15	0.9973	0.9867	-3356.9	-1946.1	-0.0	25.0	17.98	56.27
0.20	0.9964	0.9824	-3179.4	-1941.9	-0.1	33.7	17.98	56.37
0.30	0.9947	0.9737	-2929.8	-1933.3	-0.1	51.2	17.98	56.55
0.40	0.9929	0.9652	-2753.5	-1924.6	-0.3	69.3	17.98	56.68
0.50	0.9912	0.9568	-2617.4	-1915.7	-0.4	87.8	17.98	56.78
0.60	0.9895	0.9485	-2506.7	-1906.6	-0.6	106.6	17.98	56.85
0.70	0.9878	0.9403	-2413.5	-1897.4	-0.8	125.9	17.98	56.88
0.80	0.9862	0.9322	-2333.1	-1888.1	-1.1	145.5	17.98	56.88
0.90	0.9845	0.9242	-2262.6	-1878.6	-1.4	165.5	17.98	56.84
1.00	0.9829	0.9162	-2199.7	-1869.1	-1.7	185.8	17.98	56.78
1.20	0.9797	0.9007	-2091.7	-1849.6	-2.6	227.2	17.98	56.57
1.40	0.9766	0.8856	-2001.1	-1829.7	-3.6	269.7	17.99	56.26
1.60	0.9735	0.8709	-1923.3	-1809.4	-4.7	312.9	18.00	55.85
1.80	0.9705	0.8565	-1855.4	-1788.7	-6.1	356.9	18.02	55.36
2.00	0.9676	0.8424	-1795.1	-1767.8	-7.6	401.4	18.04	54.80
2.50	0.9605	0.8088	-1669.3	-1714.4	-12.2	514.1	18.11	53.10
3.00	0.9537	0.7773	-1568.7	-1660.0	-17.8	627.5	18.21	51.10
4.00	0.9413	0.7196	-1414.9	-1549.7	-31.8	850.3	18.49	46.56
5.00	0.9300	0.6685	-1300.6	-1440.2	-48.7	1059.4	18.88	41.82
6.00	0.9198	0.6230	-1211.0	-1334.0	-67.4	1248.0	19.32	37.36
7.00	0.9105	0.5824	-1138.2	-1232.9	-86.5	1411.4	19.77	33.51
8.00	0.9020	0.5461	-1077.6	-1138.4	-104.7	1546.7	20.17	30.49
9.00	0.8943	0.5136	-1026.1	-1051.5	-120.9	1652.6	20.48	28.47
10.00	0.8872	0.4843	-981.7	-972.9	-133.8	1728.5	20.64	27.51
12.00	0.8746	0.4341	-908.9	-842.2	-146.2	1792.8	20.35	28.92
14.00	0.8641	0.3919	-851.0	-745.3	-162.0	1855.6	20.23	29.61
16.00	0.8554	0.3560	-804.4	-660.8	-179.0	1918.8	20.50	28.60
18.00	0.8479	0.3257	-765.9	-589.2	-192.4	1962.7	20.73	27.85
20.00	0.8413	0.2999	-733.5	-528.3	-202.6	1992.4	20.92	27.30
30.00	0.8145	0.2152	-625.7	-331.5	-216.4	2027.4	21.36	26.26
40.00	0.7895	0.1696	-562.6	-234.6	-197.7	1998.2	21.28	26.37
50.00	0.7626	0.1416	-519.1	-183.2	-170.9	1965.1	20.99	26.73
60.00	0.7336	0.1227	-485.8	-153.8	-146.5	1940.3	20.64	27.08
80.00	0.6740	0.0985	-435.8	-123.6	-115.5	1915.0	20.01	27.59
100.00	0.6171	0.0832	-398.2	-108.4	-105.8	1908.9	19.54	27.88
150.00	0.5012	0.0609	-332.0	-87.7	-127.5	1918.0	18.92	28.17
200.00	0.4191	0.0484	-287.5	-74.3	-165.6	1930.2	18.66	28.26
INF	0.0000	0.0000	0.0	0.0	-359.6	1958.5	17.50	28.36

* STANDARD STATE VALUES
JUNE 12,1970,

TABLE 10

THERMODYNAMIC PROPERTIES OF THE SYSTEM *n*-PROPANOL–WATER AT 10°C

Molality m	Activity of solvent a_1	Act.Coeff. of solute γ_2	Gibbs Energy of solution ΔG_S cal mol^{-1}	Heat of solution ΔH_S cal mol^{-1}	Partial Molal Enthalpy solvent, $\overline{L}_1$ cal mol^{-1}	Partial Molal Enthalpy solute, $\overline{L}_2$ cal mol^{-1}	Partial Molal Heat Capacity solvent, $\overline{C}_1$ cal deg^{-1} mol^{-1}	Partial Molal Heat Capacity solute, $\overline{C}_2$ cal deg^{-1} mol^{-1}
0.00	1.0000	1.0000	-972.9*	-3047.5*	0.0	0.0	18.06	85.17
0.02	0.9996	0.9975	-3736.3	-3048.1	0.0	-1.1	18.06	85.61
0.05	0.9991	0.9938	-3222.7	-3048.8	0.0	-2.3	18.06	86.24
0.10	0.9982	0.9877	-2834.7	-3049.5	0.0	-2.9	18.06	87.23
0.15	0.9973	0.9817	-2608.1	-3049.7	-0.0	-2.0	18.06	88.16
0.20	0.9964	0.9759	-2448.1	-3049.4	-0.0	0.6	18.06	89.03
0.30	0.9947	0.9645	-2223.3	-3047.1	-0.1	10.1	18.05	90.57
0.40	0.9930	0.9536	-2064.8	-3042.9	-0.1	25.4	18.04	91.89
0.50	0.9913	0.9430	-1942.5	-3036.8	-0.3	46.1	18.03	92.97
0.60	0.9896	0.9328	-1843.1	-3028.8	-0.6	72.0	18.02	93.85
0.70	0.9880	0.9230	-1759.5	-3019.0	-0.9	102.8	18.02	94.52
0.80	0.9863	0.9135	-1687.4	-3007.6	-1.4	138.1	18.01	94.99
0.90	0.9847	0.9043	-1624.3	-2994.5	-2.0	177.7	18.01	95.28
1.00	0.9831	0.8953	-1568.0	-2979.9	-2.8	221.4	18.00	95.39
1.20	0.9799	0.8782	-1471.3	-2946.2	-4.7	319.9	18.01	95.13
1.40	0.9768	0.8620	-1390.3	-2907.2	-7.3	431.6	18.03	94.27
1.60	0.9738	0.8466	-1320.7	-2863.2	-10.7	554.6	18.07	92.89
1.80	0.9708	0.8318	-1259.9	-2814.8	-14.7	687.2	18.12	91.04
2.00	0.9679	0.8177	-1206.0	-2762.4	-19.6	827.8	18.20	88.78
2.50	0.9608	0.7843	-1093.3	-2616.7	-34.8	1204.2	18.49	81.72
3.00	0.9541	0.7528	-1003.3	-2455.0	-54.4	1599.3	18.91	73.25
4.00	0.9420	0.6928	-865.7	-2105.1	-103.2	2375.0	20.08	54.65
5.00	0.9320	0.6334	-764.4	-1749.5	-156.9	3039.7	21.49	37.27
6.00	0.9245	0.5731	-686.8	-1416.6	-203.5	3513.5	22.78	24.14
7.00	0.9201	0.5119	-626.5	-1128.1	-230.1	3743.8	23.57	17.34
8.00	0.9194	0.4506	-579.6	-899.9	-223.6	3699.1	23.44	18.21
9.00	0.9229	0.3907	-543.8	-743.4	-171.7	3363.3	22.00	27.51
10.00	0.9279	0.3409	-516.5	-658.6	-102.2	2956.4	20.15	38.54
12.00	0.9246	0.2892	-476.6	-555.1	-122.2	3057.6	20.56	36.46
14.00	0.9224	0.2505	-447.0	-469.0	-138.6	3128.1	20.91	34.99
16.00	0.9207	0.2207	-424.3	-397.1	-151.5	3176.0	21.18	33.96
18.00	0.9193	0.1971	-406.2	-336.8	-161.1	3207.4	21.40	33.25
20.00	0.9179	0.1782	-391.4	-286.1	-167.6	3226.7	21.56	32.78
30.00	0.9087	0.1215	-344.8	-127.4	-168.5	3231.8	21.84	32.10
40.00	0.8944	0.0934	-318.2	-54.3	-143.3	3192.1	21.75	32.23
50.00	0.8765	0.0766	-299.3	-18.3	-113.7	3155.4	21.68	32.33
60.00	0.8566	0.0654	-284.5	0.4	-87.7	3129.0	21.71	32.30
80.00	0.8149	0.0510	-261.4	16.6	-52.6	3100.5	22.09	32.00
100.00	0.7738	0.0421	-243.6	22.6	-34.5	3089.2	22.65	31.66
150.00	0.6806	0.0298	-211.1	27.4	-19.0	3081.9	23.88	31.09
200.00	0.6028	0.0232	-188.1	28.8	-9.4	3078.9	24.45	30.91
INF	0.0000	0.0000	0.0	0.0	429.7	3047.5	12.53	31.60

* STANDARD STATE VALUES
JUNE 24,1970,

TABLE 11

THERMODYNAMIC PROPERTIES OF THE SYSTEM *n*-PROPANOL–WATER AT 25°C

Molality m	Activity of solvent a_1	Act.Coeff. of solute γ_2	Gibbs Energy of solution ΔG_S cal mol^{-1}	Heat of solution ΔH_S cal mol^{-1}	Partial Molal Enthalpy		Partial Molal Heat Capacity	
					solvent, $\bar{L}_1$ cal mol^{-1}	solute, $\bar{L}_2$ cal mol^{-1}	solvent, $\bar{C}_1$ cal deg^{-1} mol^{-1}	solute, $\bar{C}_2$
0.00	1.0000	1.0000	-883.2*	-2286.1*	0.0	0.0	18.00	81.65
0.02	0.9996	0.9973	-3792.9	-2283.8	-0.0	4.7	18.00	81.99
0.05	0.9991	0.9933	-3252.2	-2280.2	-0.0	12.0	18.00	82.49
0.10	0.9982	0.9867	-2843.8	-2274.0	-0.0	24.7	18.00	83.27
0.15	0.9973	0.9801	-2605.4	-2267.6	-0.1	38.1	17.99	84.01
0.20	0.9965	0.9735	-2437.1	-2260.9	-0.1	52.3	17.99	84.69
0.30	0.9947	0.9605	-2200.9	-2246.9	-0.2	82.5	17.99	85.90
0.40	0.9930	0.9475	-2034.4	-2232.1	-0.4	115.4	17.98	86.93
0.50	0.9913	0.9347	-1906.2	-2216.3	-0.7	150.6	17.97	87.77
0.60	0.9897	0.9219	-1802.2	-2199.8	-1.1	188.0	17.97	88.44
0.70	0.9881	0.9093	-1714.9	-2182.4	-1.6	227.6	17.96	88.94
0.80	0.9865	0.8969	-1639.9	-2164.4	-2.1	269.0	17.96	89.29
0.90	0.9849	0.8845	-1574.2	-2145.6	-2.8	312.3	17.95	89.49
1.00	0.9834	0.8723	-1515.8	-2126.2	-3.6	357.3	17.95	89.54
1.20	0.9804	0.8483	-1416.0	-2085.5	-5.4	451.6	17.96	89.25
1.40	0.9775	0.8248	-1332.8	-2042.6	-7.8	551.1	17.98	88.49
1.60	0.9747	0.8019	-1262.0	-1997.7	-10.6	654.8	18.01	87.30
1.80	0.9720	0.7796	-1200.5	-1951.1	-13.8	761.8	18.06	85.73
2.00	0.9695	0.7578	-1146.3	-1902.9	-17.6	871.3	18.12	83.84
2.50	0.9636	0.7059	-1034.9	-1777.5	-28.9	1150.7	18.36	77.96
3.00	0.9583	0.6576	-947.8	-1647.1	-42.7	1429.7	18.71	70.95
4.00	0.9496	0.5713	-819.1	-1382.8	-75.5	1951.3	19.67	55.66
5.00	0.9431	0.4977	-728.5	-1128.5	-110.0	2378.9	20.82	41.42
6.00	0.9386	0.4354	-661.6	-898.3	-139.0	2673.9	21.88	30.71
7.00	0.9358	0.3828	-610.8	-702.8	-154.9	2812.0	22.52	25.19
8.00	0.9346	0.3384	-571.4	-549.4	-150.3	2779.5	22.40	25.96
9.00	0.9345	0.3009	-540.4	-443.5	-118.1	2571.1	21.22	33.63
10.00	0.9352	0.2694	-516.3	-381.5	-73.4	2312.1	19.75	42.38
12.00	0.9334	0.2267	-479.0	-307.3	-87.5	2383.5	20.12	40.47
14.00	0.9323	0.1953	-451.8	-245.8	-98.9	2432.3	20.45	39.06
16.00	0.9315	0.1714	-431.1	-194.6	-107.6	2464.7	20.74	38.01
18.00	0.9307	0.1528	-414.8	-151.9	-113.7	2484.9	20.98	37.23
20.00	0.9298	0.1379	-401.6	-116.2	-117.6	2496.2	21.17	36.65
30.00	0.9203	0.0940	-359.7	-7.1	-112.1	2486.5	21.73	35.34
40.00	0.9038	0.0726	-334.8	39.7	-86.0	2445.2	21.94	35.00
50.00	0.8833	0.0597	-316.5	59.7	-55.9	2407.9	22.08	34.83
60.00	0.8612	0.0511	-301.6	67.6	-28.5	2380.1	22.24	34.67
80.00	0.8164	0.0400	-277.8	69.6	12.7	2346.9	22.68	34.33
100.00	0.7736	0.0331	-259.1	66.0	38.7	2330.6	23.18	34.02
150.00	0.6788	0.0234	-224.7	55.8	71.2	2315.6	24.21	33.54
200.00	0.6003	0.0182	-200.4	48.4	89.0	2309.8	24.74	33.37
INF	0.0000	0.0000	0.0	0.0	388.8	2286.1	18.08	33.70

* STANDARD STATE VALUES
JUNE 24,1970,

TABLE 12

THERMODYNAMIC PROPERTIES OF THE SYSTEM *n*-PROPANOL–WATER AT 40°C

Molality m	Activity of solvent a_1	Act.Coeff. of solute γ_2	Gibbs Energy of solution ΔG_S cal mol^{-1}	Heat of solution ΔH_S cal mol^{-1}	Partial Molal Enthalpy		Partial Molal Heat Capacity	
					solvent, $\bar{L}_1$ cal mol^{-1}	solute, $\bar{L}_2$ cal mol^{-1}	solvent, $\bar{C}_1$ cal deg^{-1} mol^{-1}	solute, $\bar{C}_2$
0.00	1.0000	1.0000	-829.7*	-1609.1*	-0.0	0.0	17.98	78.42
0.02	0.9996	0.9968	-3886.1	-1604.6	-0.0	9.2	17.98	78.67
0.05	0.9991	0.9919	-3318.4	-1597.7	-0.0	22.9	17.98	79.04
0.10	0.9982	0.9839	-2889.9	-1586.2	-0.0	45.9	17.98	79.61
0.15	0.9973	0.9759	-2640.0	-1574.7	-0.1	68.8	17.98	80.15
0.20	0.9965	0.9678	-2463.6	-1563.3	-0.2	91.8	17.98	80.65
0.30	0.9947	0.9519	-2216.4	-1540.3	-0.4	137.8	17.97	81.53
0.40	0.9931	0.9361	-2042.6	-1517.3	-0.7	183.9	17.97	82.27
0.50	0.9914	0.9203	-1908.9	-1494.3	-1.0	229.9	17.97	82.87
0.60	0.9898	0.9047	-1800.7	-1471.3	-1.5	275.8	17.96	83.33
0.70	0.9882	0.8893	-1710.0	-1448.3	-2.0	321.7	17.96	83.67
0.80	0.9867	0.8740	-1632.2	-1425.3	-2.6	367.4	17.95	83.89
0.90	0.9851	0.8589	-1564.3	-1402.4	-3.3	412.9	17.95	83.99
1.00	0.9837	0.8439	-1504.1	-1379.5	-4.1	458.2	17.95	83.99
1.20	0.9808	0.8146	-1401.4	-1333.9	-5.9	548.2	17.96	83.68
1.40	0.9781	0.7860	-1316.3	-1288.6	-8.0	636.9	17.97	83.00
1.60	0.9755	0.7583	-1244.1	-1243.6	-10.3	724.1	18.00	82.01
1.80	0.9731	0.7315	-1181.8	-1199.0	-13.0	809.7	18.04	80.72
2.00	0.9708	0.7055	-1127.2	-1154.8	-15.8	893.5	18.09	79.19
2.50	0.9656	0.6446	-1016.1	-1046.7	-23.9	1093.6	18.28	74.50
3.00	0.9612	0.5893	-930.5	-942.6	-33.1	1278.6	18.56	68.96
4.00	0.9545	0.4949	-806.9	-748.4	-52.9	1595.5	19.32	56.97
5.00	0.9501	0.4196	-722.4	-576.3	-72.1	1833.0	20.21	45.87
6.00	0.9473	0.3604	-661.7	-429.0	-87.0	1985.3	21.03	37.57
7.00	0.9454	0.3141	-616.4	-308.3	-94.5	2050.2	21.52	33.34
8.00	0.9439	0.2781	-581.3	-215.1	-91.4	2028.5	21.42	34.01
9.00	0.9422	0.2502	-553.2	-149.7	-75.2	1923.0	20.48	40.06
10.00	0.9398	0.2285	-529.8	-106.7	-49.7	1778.3	19.39	46.52
12.00	0.9389	0.1914	-493.8	-56.7	-58.4	1822.5	19.74	44.79
14.00	0.9384	0.1644	-467.7	-16.0	-64.9	1850.6	20.05	43.43
16.00	0.9381	0.1440	-448.1	17.3	-69.3	1867.0	20.34	42.36
18.00	0.9377	0.1282	-432.7	44.5	-71.7	1874.9	20.60	41.51
20.00	0.9369	0.1157	-420.3	66.8	-72.4	1876.8	20.84	40.82
30.00	0.9265	0.0790	-380.5	129.3	-56.4	1842.8	21.68	38.89
40.00	0.9078	0.0612	-356.1	149.1	-24.9	1792.8	22.18	38.07
50.00	0.8849	0.0505	-337.4	151.6	8.8	1751.0	22.53	37.64
60.00	0.8608	0.0433	-321.8	147.3	39.6	1719.8	22.82	37.35
80.00	0.8131	0.0340	-296.6	132.7	87.8	1680.9	23.32	36.95
100.00	0.7687	0.0281	-276.4	118.3	120.8	1660.4	23.76	36.68
150.00	0.6725	0.0199	-239.4	91.7	167.3	1638.9	24.59	36.29
200.00	0.5938	0.0156	-213.3	75.0	193.0	1630.6	25.09	36.13
INF	0.0000	0.0000	0.0	0.0	432.2	1609.1	23.68	36.10

* STANDARD STATE VALUES
JUNE 24,1970,

TABLE 13

THERMODYNAMIC PROPERTIES OF THE SYSTEM *iso*-PROPANOL–WATER AT 10°C

Molality m	Activity of solvent a_1	Act.Coeff. of solute γ_2	Gibbs Energy of solution ΔG_S cal mol^{-1}	Heat of solution ΔH_S cal mol^{-1}	Partial Molal Enthalpy solvent, $\overline{L}_1$ cal mol^{-1}	solute, $\overline{L}_2$ cal mol^{-1}	Partial Molal Heat Capacity solvent, $\overline{C}_1$ cal deg^{-1} mol^{-1}	solute, $\overline{C}_2$
0.00	1.0000	1.0000	-1397.4*	-3874.5*	0.0	0.0	18.06	79.56
0.02	0.9996	1.0000	-4160.0	-3875.6	0.0	-2.1	18.06	79.94
0.05	0.9991	1.0001	-3645.3	-3877.0	0.0	-4.7	18.06	80.50
0.10	0.9982	1.0003	-3255.5	-3878.9	0.0	-7.8	18.06	81.41
0.15	0.9973	1.0006	-3027.2	-3880.4	0.0	-9.5	18.06	82.28
0.20	0.9964	1.0009	-2865.4	-3881.4	0.0	-9.7	18.06	83.11
0.30	0.9946	1.0016	-2637.1	-3881.8	-0.0	-5.9	18.05	84.67
0.40	0.9928	1.0024	-2475.0	-3880.4	-0.1	3.3	18.04	86.09
0.50	0.9910	1.0035	-2349.2	-3877.3	-0.2	17.6	18.03	87.38
0.60	0.9892	1.0046	-2246.4	-3872.3	-0.4	36.9	18.02	88.53
0.70	0.9874	1.0059	-2159.4	-3865.7	-0.7	60.8	18.01	89.57
0.80	0.9856	1.0073	-2083.9	-3857.5	-1.0	89.2	17.99	90.48
0.90	0.9838	1.0088	-2017.4	-3847.7	-1.5	121.8	17.98	91.28
1.00	0.9820	1.0104	-1957.7	-3836.4	-2.2	158.4	17.97	91.97
1.20	0.9784	1.0138	-1854.4	-3809.5	-3.8	242.6	17.95	93.04
1.40	0.9748	1.0173	-1766.9	-3777.3	-6.1	340.4	17.93	93.71
1.60	0.9712	1.0210	-1690.9	-3740.2	-9.1	450.1	17.93	94.03
1.80	0.9676	1.0246	-1623.7	-3698.5	-12.8	570.3	17.93	94.02
2.00	0.9640	1.0282	-1563.5	-3652.7	-17.2	699.7	17.94	93.70
2.50	0.9551	1.0365	-1435.7	-3522.3	-31.6	1054.6	18.02	91.78
3.00	0.9462	1.0427	-1330.9	-3373.4	-50.8	1440.3	18.18	88.54
4.00	0.9292	1.0459	-1165.5	-3038.3	-101.4	2243.7	18.76	79.35
5.00	0.9136	1.0323	-1038.4	-2678.9	-163.5	3010.4	19.66	68.32
6.00	0.9002	0.9996	-936.8	-2319.6	-228.6	3669.6	20.77	57.07
7.00	0.8896	0.9480	-854.3	-1979.5	-287.2	4172.7	21.98	46.76
8.00	0.8826	0.8798	-786.7	-1673.0	-329.6	4488.4	23.12	38.24
9.00	0.8798	0.7992	-731.7	-1410.8	-346.1	4598.4	24.07	32.07
10.00	0.8815	0.7111	-687.4	-1200.7	-328.1	4494.7	24.65	28.60
12.00	0.9011	0.5314	-626.1	-956.1	-157.8	3648.4	24.24	30.49
14.00	0.8897	0.4791	-587.2	-843.1	-198.1	3816.9	22.33	39.24
16.00	0.8826	0.4319	-553.5	-739.4	-220.7	3901.0	22.68	37.95
18.00	0.8760	0.3933	-525.6	-650.7	-239.4	3962.0	22.92	37.15
20.00	0.8700	0.3612	-502.1	-574.6	-254.3	4005.6	23.08	36.69
30.00	0.8447	0.2575	-422.7	-322.2	-285.3	4080.1	23.04	36.72
40.00	0.8244	0.2008	-375.8	-191.6	-274.4	4063.7	22.56	37.48
50.00	0.8069	0.1650	-344.1	-118.6	-248.4	4031.7	22.27	37.85
60.00	0.7911	0.1403	-320.8	-75.2	-219.9	4002.8	22.30	37.82
80.00	0.7610	0.1085	-288.0	-29.7	-171.3	3963.7	23.17	37.14
100.00	0.7309	0.0890	-265.2	-8.3	-136.9	3942.2	24.55	36.29
150.00	0.6536	0.0624	-227.7	12.6	-87.5	3919.5	27.90	34.77
200.00	0.5802	0.0486	-202.7	19.4	-57.5	3909.8	30.02	34.08
INF	0.0000	0.0000	0.0	0.0	369.5	3874.5	17.49	34.38

* STANDARD STATE VALUES
JULY 7,1970,

TABLE 14

THERMODYNAMIC PROPERTIES OF THE SYSTEM *iso*-PROPANOL–WATER AT 25°C

Molality m	Activity of solvent a_1	Act.Coeff. of solute γ_2	Gibbs Energy of solution ΔG_S cal mol^{-1}	Heat of solution ΔH_S cal mol^{-1}	Partial Molal Enthalpy		Partial Molal Heat Capacity	
					solvent, $\bar{L}_1$ cal mol^{-1}	solute, $\bar{L}_2$ cal mol^{-1}	solvent, $\bar{C}_1$ cal deg^{-1} mol^{-1}	solute, $\bar{C}_2$
0.00	1.0000	1.0000	-1283.9*	-3191.8*	0.0	0.0	18.00	82.80
0.02	0.9996	1.0000	-4192.9	-3190.2	-0.0	3.2	18.00	83.11
0.05	0.9991	1.0000	-3650.9	-3187.7	-0.0	8.2	18.00	83.57
0.10	0.9982	0.9999	-3240.6	-3183.4	-0.0	17.4	18.00	84.31
0.15	0.9973	0.9997	-3000.3	-3178.7	-0.0	27.5	17.99	85.00
0.20	0.9964	0.9995	-2830.0	-3173.8	-0.1	38.5	17.99	85.67
0.30	0.9946	0.9989	-2589.9	-3162.9	-0.2	63.1	17.99	86.88
0.40	0.9928	0.9981	-2419.6	-3150.9	-0.4	91.0	17.98	87.96
0.50	0.9911	0.9971	-2287.6	-3137.9	-0.6	122.1	17.97	88.90
0.60	0.9893	0.9958	-2179.8	-3123.7	-1.0	156.2	17.96	89.72
0.70	0.9875	0.9944	-2088.8	-3108.5	-1.4	193.1	17.96	90.42
0.80	0.9858	0.9927	-2010.0	-3092.3	-1.9	232.6	17.95	91.00
0.90	0.9840	0.9909	-1940.6	-3075.2	-2.6	274.7	17.94	91.46
1.00	0.9823	0.9888	-1878.6	-3057.2	-3.3	319.2	17.94	91.82
1.20	0.9788	0.9841	-1771.6	-3018.6	-5.2	414.6	17.93	92.24
1.40	0.9754	0.9786	-1681.4	-2976.8	-7.6	517.7	17.93	92.29
1.60	0.9721	0.9725	-1603.5	-2932.2	-10.6	627.6	17.93	91.99
1.80	0.9688	0.9657	-1535.2	-2884.9	-14.1	743.2	17.95	91.38
2.00	0.9656	0.9582	-1474.4	-2835.3	-18.3	863.5	17.98	90.50
2.50	0.9578	0.9372	-1346.7	-2702.6	-31.1	1179.7	18.12	87.25
3.00	0.9504	0.9130	-1244.2	-2560.2	-47.4	1508.0	18.34	82.85
4.00	0.9372	0.8578	-1087.0	-2258.9	-88.5	2160.6	19.03	71.93
5.00	0.9260	0.7965	-970.9	-1952.5	-136.5	2755.1	19.99	59.99
6.00	0.9171	0.7325	-881.4	-1657.3	-184.9	3245.3	21.11	48.71
7.00	0.9104	0.6684	-810.7	-1385.8	-226.3	3600.2	22.21	39.27
8.00	0.9060	0.6062	-754.1	-1147.3	-253.2	3801.1	23.13	32.48
9.00	0.9039	0.5472	-708.4	-948.5	-258.6	3837.8	23.67	28.88
10.00	0.9040	0.4922	-671.5	-794.2	-236.0	3707.3	23.69	28.77
12.00	0.9107	0.3954	-617.6	-629.7	-85.0	2955.3	21.52	39.46
14.00	0.9033	0.3499	-581.4	-553.4	-142.4	3202.8	21.16	41.24
16.00	0.8976	0.3133	-550.6	-478.4	-160.6	3270.5	21.40	40.34
18.00	0.8924	0.2839	-525.3	-413.6	-176.2	3321.6	21.56	39.81
20.00	0.8874	0.2598	-504.0	-357.2	-189.2	3359.6	21.66	39.53
30.00	0.8640	0.1839	-432.1	-165.6	-221.3	3435.6	21.56	39.69
40.00	0.8427	0.1436	-388.9	-63.3	-216.5	3428.9	21.22	40.23
50.00	0.8231	0.1183	-358.9	-5.9	-193.6	3400.9	21.10	40.39
60.00	0.8048	0.1008	-336.4	27.4	-163.6	3370.5	21.27	40.23
80.00	0.7705	0.0783	-304.0	58.6	-101.0	3320.5	22.26	39.45
100.00	0.7370	0.0644	-280.9	69.0	-46.0	3286.3	23.62	38.61
150.00	0.6548	0.0453	-241.9	68.9	51.6	3241.6	26.70	37.20
200.00	0.5789	0.0353	-215.6	61.5	111.4	3222.3	28.56	36.60
INF	0.0000	0.0000	0.0	0.0	356.3	3191.8	16.79	36.94

* STANDARD STATE VALUES
JULY 7,1970,

TABLE 15

THERMODYNAMIC PROPERTIES OF THE SYSTEM *iso*-PROPANOL–WATER AT 40°C

Molality m	Activity of solvent a_1	Act.Coeff. of solute γ_2	Gibbs Energy of solution ΔG_S cal mol^{-1}	Heat of solution ΔH_S cal mol^{-1}	Partial Molal Enthalpy		Partial Molal Heat Capacity	
					solvent, $\bar{L}_1$ cal mol^{-1}	solute, $\bar{L}_2$ cal mol^{-1}	solvent, $\bar{C}_1$ cal deg^{-1}	solute, $\bar{C}_2$ mol^{-1}
0.00	1.0000	1.0000	-1205.0*	-2498.8*	0.0	0.0	17.98	86.80
0.02	0.9996	0.9996	-4260.4	-2495.1	-0.0	7.4	17.98	87.05
0.05	0.9991	0.9989	-3691.5	-2489.5	-0.0	18.5	17.98	87.40
0.10	0.9982	0.9977	-3260.8	-2480.2	-0.0	37.4	17.98	87.96
0.15	0.9973	0.9963	-3008.8	-2470.7	-0.1	56.7	17.98	88.49
0.20	0.9964	0.9949	-2830.3	-2461.1	-0.1	76.3	17.98	88.98
0.30	0.9946	0.9917	-2578.8	-2441.5	-0.3	116.6	17.97	89.85
0.40	0.9929	0.9881	-2400.8	-2421.5	-0.6	158.1	17.97	90.59
0.50	0.9911	0.9841	-2263.0	-2401.1	-0.9	200.8	17.97	91.19
0.60	0.9894	0.9797	-2150.7	-2380.3	-1.4	244.6	17.96	91.67
0.70	0.9876	0.9751	-2056.0	-2359.1	-1.9	289.4	17.96	92.03
0.80	0.9859	0.9701	-1974.2	-2337.5	-2.5	335.1	17.95	92.27
0.90	0.9842	0.9647	-1902.3	-2315.6	-3.2	381.7	17.95	92.41
1.00	0.9826	0.9591	-1838.2	-2293.4	-4.0	429.1	17.95	92.44
1.20	0.9793	0.9471	-1727.9	-2248.1	-6.0	525.9	17.96	92.21
1.40	0.9761	0.9342	-1635.4	-2201.7	-8.3	625.0	17.97	91.62
1.60	0.9730	0.9204	-1556.0	-2154.4	-11.0	725.8	17.99	90.71
1.80	0.9699	0.9059	-1486.6	-2106.4	-14.1	827.8	18.03	89.51
2.00	0.9670	0.8908	-1425.2	-2057.7	-17.6	930.6	18.08	88.05
2.50	0.9601	0.8511	-1297.7	-1934.0	-28.1	1188.2	18.27	83.48
3.00	0.9538	0.8098	-1196.7	-1808.9	-40.6	1441.8	18.54	77.92
4.00	0.9432	0.7267	-1045.5	-1560.3	-70.6	1917.5	19.34	65.26
5.00	0.9351	0.6478	-937.3	-1322.3	-103.6	2326.2	20.38	52.42
6.00	0.9290	0.5765	-856.4	-1102.6	-135.2	2647.0	21.50	41.12
7.00	0.9248	0.5141	-793.9	-907.0	-160.8	2866.8	22.50	32.54
8.00	0.9219	0.4605	-744.7	-739.4	-175.8	2978.9	23.18	27.49
9.00	0.9199	0.4151	-705.2	-602.8	-175.9	2980.8	23.33	26.45
10.00	0.9185	0.3771	-672.8	-498.8	-157.4	2873.7	22.77	29.69
12.00	0.9155	0.3194	-623.1	-391.4	-52.1	2348.2	18.85	49.19
14.00	0.9122	0.2768	-588.6	-338.4	-103.3	2570.0	20.03	43.99
16.00	0.9078	0.2466	-559.5	-283.4	-118.8	2627.3	20.16	43.50
18.00	0.9035	0.2226	-535.8	-235.0	-132.5	2672.4	20.24	43.23
20.00	0.8993	0.2031	-515.9	-192.3	-144.5	2707.5	20.28	43.12
30.00	0.8780	0.1429	-448.9	-41.9	-178.4	2787.0	20.13	43.43
40.00	0.8561	0.1116	-408.2	41.5	-177.6	2786.7	19.94	43.75
50.00	0.8347	0.0921	-379.3	88.3	-155.4	2759.5	19.98	43.70
60.00	0.8141	0.0787	-357.2	114.3	-121.7	2725.6	20.29	43.39
80.00	0.7748	0.0614	-324.3	134.3	-43.5	2663.2	21.40	42.52
100.00	0.7373	0.0507	-300.3	135.4	31.8	2616.5	22.74	41.69
150.00	0.6486	0.0358	-258.9	117.1	173.7	2551.6	25.55	40.40
200.00	0.5700	0.0280	-230.6	97.2	259.3	2524.0	27.15	39.89
INF	0.0000	0.0000	0.0	0.0	333.4	2498.8	16.14	40.26

* STANDARD STATE VALUES
JULY 7,1970,

TABLE 16

THERMODYNAMIC PROPERTIES OF THE SYSTEM *n*-BUTANOL–WATER AT 10°C

Molality m	Activity of solvent a_1	Act.Coeff. of solute γ_2	Gibbs Energy of solution ΔG_S cal mol^{-1}	Heat of solution ΔH_S cal mol^{-1}	Partial Molal Enthalpy solvent, $\overline{L}_1$ cal mol^{-1}	 solute, $\overline{L}_2$ cal mol^{-1}	Partial Molal Heat Capacity solvent, $\overline{C}_1$ cal deg^{-1}	 solute, $\overline{C}_2$ mol^{-1}
0.00	1.0000	1.0000	-196.0*	-3058.9*	0.0	0.0	18.06	105.31
0.02	0.9996	1.0017	-2958.1	-3061.1	0.0	-4.1	18.06	106.03
0.05	0.9991	1.0038	-2442.8	-3063.7	0.0	-8.7	18.06	107.00
0.10	0.9982	1.0062	-2052.2	-3066.8	0.0	-12.3	18.06	108.32
0.15	0.9973	1.0073	-1823.3	-3068.2	0.0	-10.8	18.06	109.25
0.20	0.9964	1.0070	-1661.2	-3067.8	-0.0	-4.3	18.06	109.81
0.30	0.9946	1.0024	-1433.1	-3062.2	-0.1	23.7	18.06	109.81
0.40	0.9929	0.9927	-1272.3	-3049.9	-0.4	71.1	18.07	108.36
0.50	0.9912	0.9780	-1148.7	-3031.2	-1.0	137.5	18.09	105.48
0.60	0.9896	0.9588	-1049.1	-3006.0	-1.8	222.6	18.13	101.21
0.70	0.9881	0.9354	-966.3	-2974.6	-3.0	326.0	18.20	95.57
0.80	0.9868	0.9082	-896.0	-2937.0	-4.7	447.1	18.29	88.60
0.90	0.9855	0.8777	-835.5	-2893.4	-6.8	585.8	18.42	80.32
1.00	0.9844	0.8444	-782.8	-2843.7	-9.5	741.5	18.58	70.77
1.10	0.9834	0.8094	-737.6	-2789.3	-12.7	910.2	18.78	60.19
54.88	1.0348	0.0168	-221.3	-2265.1	-2454.3	3276.2	370.18	-299.07
60.00	1.9674	0.0083	-238.4	-2375.5	5118.4	-4051.6	111.95	-49.22
80.00	12.0547	0.0014	-445.1	-6098.7	27172.3	-21892.7	-681.04	590.82
100.00	27.6220	0.0007	-674.9	-10686.6	38178.5	-28819.1	-1132.46	873.92
150.00	18.8963	0.0005	-1024.0	-18092.5	36927.1	-28698.1	-1303.63	966.24
200.00	3.4258	0.0007	-1139.2	-20824.3	19222.5	-23100.2	-876.59	832.14
250.00	0.5019	0.0009	-1149.8	-21354.5	-1731.1	-17911.3	-294.09	688.09
300.00	0.0827	0.0010	-1117.5	-20936.4	-21802.0	-13843.6	292.32	569.30
INF	0.0000	0.0000	0.0	0.0	-248142.0	3058.9	7543.08	40.03

* STANDARD STATE VALUES
JULY 7,1970

TABLE 17

THERMODYNAMIC PROPERTIES OF THE SYSTEM *n*-BUTANOL–WATER AT 25°C

Molality m	Activity of solvent a_1	Act.Coeff. of solute γ_2	Gibbs Energy of solution ΔG_S cal mol^{-1}	Heat of solution ΔH_S cal mol^{-1}	Partial Molal Enthalpy solvent, $\overline{L}_1$ cal mol^{-1}	solute, $\overline{L}_2$ cal mol^{-1}	Partial Molal Heat Capacity solvent, $\overline{C}_1$ cal deg^{-1}	solute, $\overline{C}_2$ mol^{-1}
0.00	1.0000	1.0000	-68.7*	-2142.9*	0.0	0.0	18.00	76.17
0.02	0.9996	1.0016	-2977.2	-2139.2	-0.0	7.5	18.00	77.00
0.05	0.9991	1.0034	-2434.7	-2133.5	-0.0	18.8	18.00	78.15
0.10	0.9982	1.0052	-2023.5	-2124.1	-0.0	37.7	17.99	79.83
0.15	0.9973	1.0054	-1782.8	-2114.6	-0.1	56.7	17.99	81.23
0.20	0.9964	1.0040	-1612.3	-2105.1	-0.1	75.7	17.99	82.33
0.30	0.9946	0.9966	-1372.7	-2086.1	-0.3	114.0	17.98	83.71
0.40	0.9929	0.9833	-1204.1	-2067.0	-0.6	152.5	17.98	83.97
0.50	0.9913	0.9645	-1075.0	-2047.8	-0.9	191.3	17.99	83.16
0.60	0.9898	0.9405	-971.2	-2028.5	-1.3	230.2	18.01	81.28
0.70	0.9883	0.9119	-885.3	-2009.2	-1.7	269.4	18.04	78.36
0.80	0.9871	0.8793	-812.7	-1989.8	-2.2	308.8	18.09	74.43
0.90	0.9859	0.8432	-750.6	-1970.3	-2.9	348.5	18.17	69.51
1.00	0.9849	0.8044	-697.0	-1950.7	-3.5	388.3	18.27	63.61
1.07	0.9844	0.7758	-663.7	-1937.0	-4.1	416.2	18.36	58.92
53.06	1.0198	0.0165	-133.7	-1862.6	-0.2	280.6	277.95	-188.69
60.00	1.2094	0.0124	-141.1	-2201.5	5701.5	-5333.1	1.88	83.03
80.00	1.6636	0.0072	-189.7	-4869.5	17284.2	-14718.8	-601.25	570.30
100.00	1.8573	0.0053	-236.9	-7663.4	22462.5	-17988.5	-926.80	774.75
150.00	1.5295	0.0039	-299.5	-11818.6	19465.7	-16878.8	-988.22	814.20
200.00	1.0118	0.0033	-312.9	-13162.1	7896.8	-13210.8	-597.13	690.95
250.00	0.6615	0.0029	-306.7	-13268.9	-4961.9	-10024.4	-100.29	568.00
300.00	0.4500	0.0026	-293.6	-12872.6	-16971.5	-7589.7	388.10	469.05
INF	0.0000	0.0000	0.0	0.0	-145545.0	2142.9	6173.19	42.31

* STANDARD STATE VALUES
JULY 7,1970

TABLE 18

THERMODYNAMIC PROPERTIES OF THE SYSTEM *n*-BUTANOL–WATER AT 40°C

Molality m	Activity of solvent a_1	Act.Coeff. of solute γ_2	Gibbs Energy of solution ΔG_S cal mol^{-1}	Heat of solution ΔH_S cal mol^{-1}	Partial Molal Enthalpy solvent, $\overline{L}_1$ cal mol^{-1}	Partial Molal Enthalpy solute, $\overline{L}_2$ cal mol^{-1}	Partial Molal Heat Capacity solvent, $\overline{C}_1$ cal deg^{-1} mol^{-1}	Partial Molal Heat Capacity solute, $\overline{C}_2$ cal deg^{-1} mol^{-1}
0.00	1.0000	1.0000	15.6*	-1353.1*	0.0	0.0	17.98	93.50
0.02	0.9996	1.0004	-3039.6	-1342.7	-0.0	20.7	17.98	94.42
0.05	0.9991	1.0006	-2470.3	-1327.5	-0.0	50.5	17.98	95.75
0.10	0.9982	0.9998	-2039.3	-1303.2	-0.1	97.5	17.98	97.80
0.15	0.9973	0.9976	-1787.2	-1280.0	-0.2	140.8	17.97	99.66
0.20	0.9964	0.9939	-1608.9	-1258.0	-0.3	180.6	17.97	101.32
0.30	0.9947	0.9825	-1358.7	-1217.6	-0.6	249.8	17.96	104.06
0.40	0.9930	0.9659	-1183.0	-1181.8	-1.0	305.2	17.94	106.05
0.50	0.9914	0.9445	-1048.6	-1150.6	-1.3	347.1	17.93	107.29
0.60	0.9899	0.9187	-940.7	-1124.0	-1.6	375.9	17.93	107.81
0.70	0.9885	0.8891	-851.4	-1101.7	-1.8	391.8	17.93	107.61
0.80	0.9872	0.8561	-776.0	-1083.8	-1.8	395.0	17.94	106.73
0.90	0.9861	0.8202	-711.6	-1070.3	-1.7	385.9	17.97	105.16
0.95	0.9855	0.8003	-681.1	-1064.8	-1.5	376.2	17.99	104.05
49.52	0.9440	0.0190	-61.3	-1034.5	1248.1	-1080.4	199.60	-98.04
50.00	0.9335	0.0191	-60.9	-1048.8	1421.9	-1274.2	184.42	-81.11
60.00	0.7527	0.0198	-41.0	-1603.7	4637.2	-4540.5	-108.15	215.74
80.00	0.5574	0.0189	21.6	-3151.4	8597.3	-7763.3	-521.43	550.24
100.00	0.4865	0.0165	78.5	-4449.6	9836.0	-8556.1	-721.11	676.03
150.00	0.5318	0.0106	161.1	-6109.6	6739.7	-7250.4	-672.78	662.62
200.00	0.7392	0.0072	189.4	-6489.8	765.8	-5349.2	-317.63	550.21
250.00	1.0674	0.0052	194.0	-6374.8	-5284.7	-3848.3	93.54	448.37
300.00	1.5035	0.0041	188.7	-6082.8	-10705.8	-2748.9	483.91	369.25
INF	0.0000	0.0000	0.0	0.0	-63514.0	1353.1	4803.29	45.05

* STANDARD STATE VALUES
JULY 7,1970

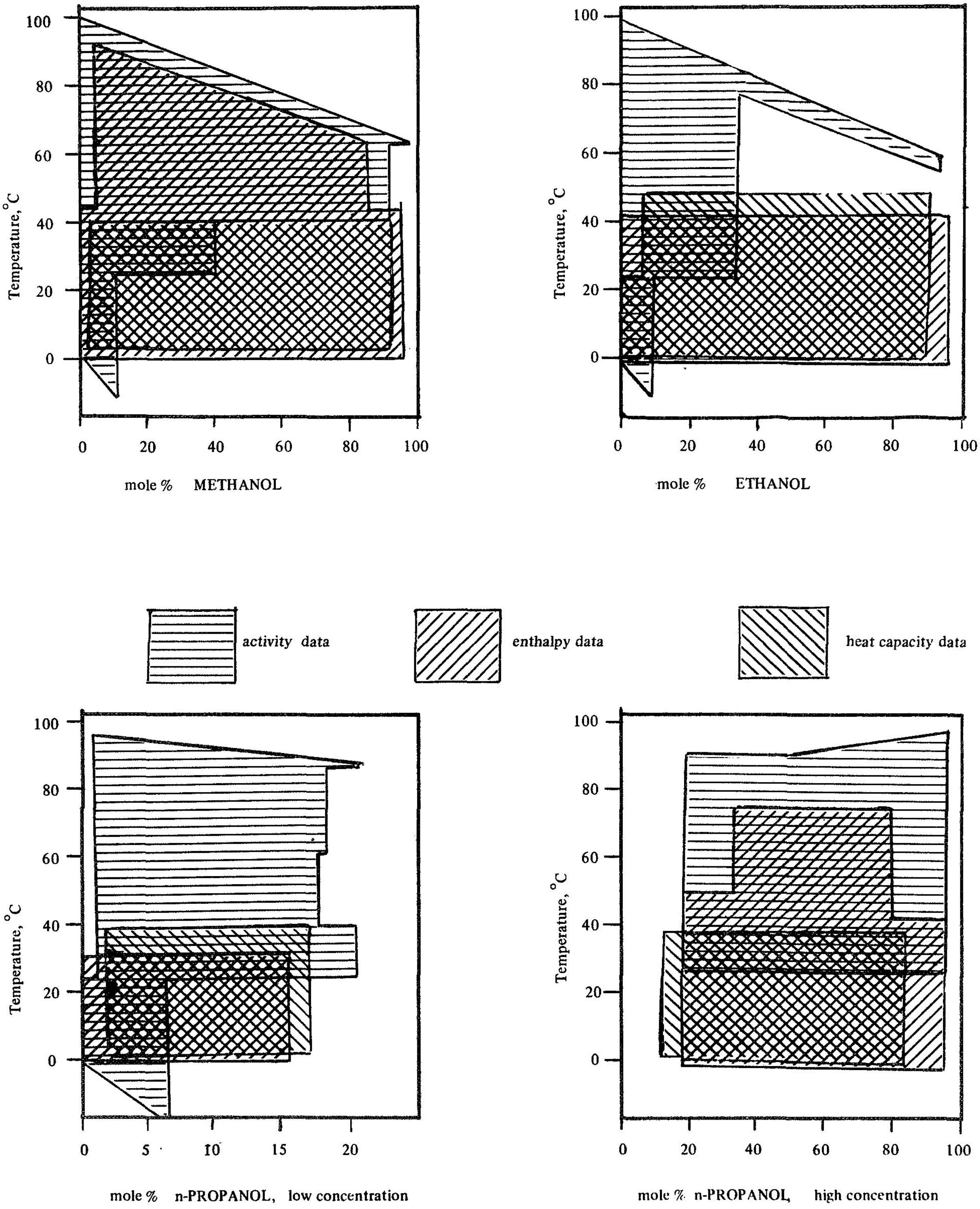

Figure 1. Temperature and Concentration Ranges of Experimental Data

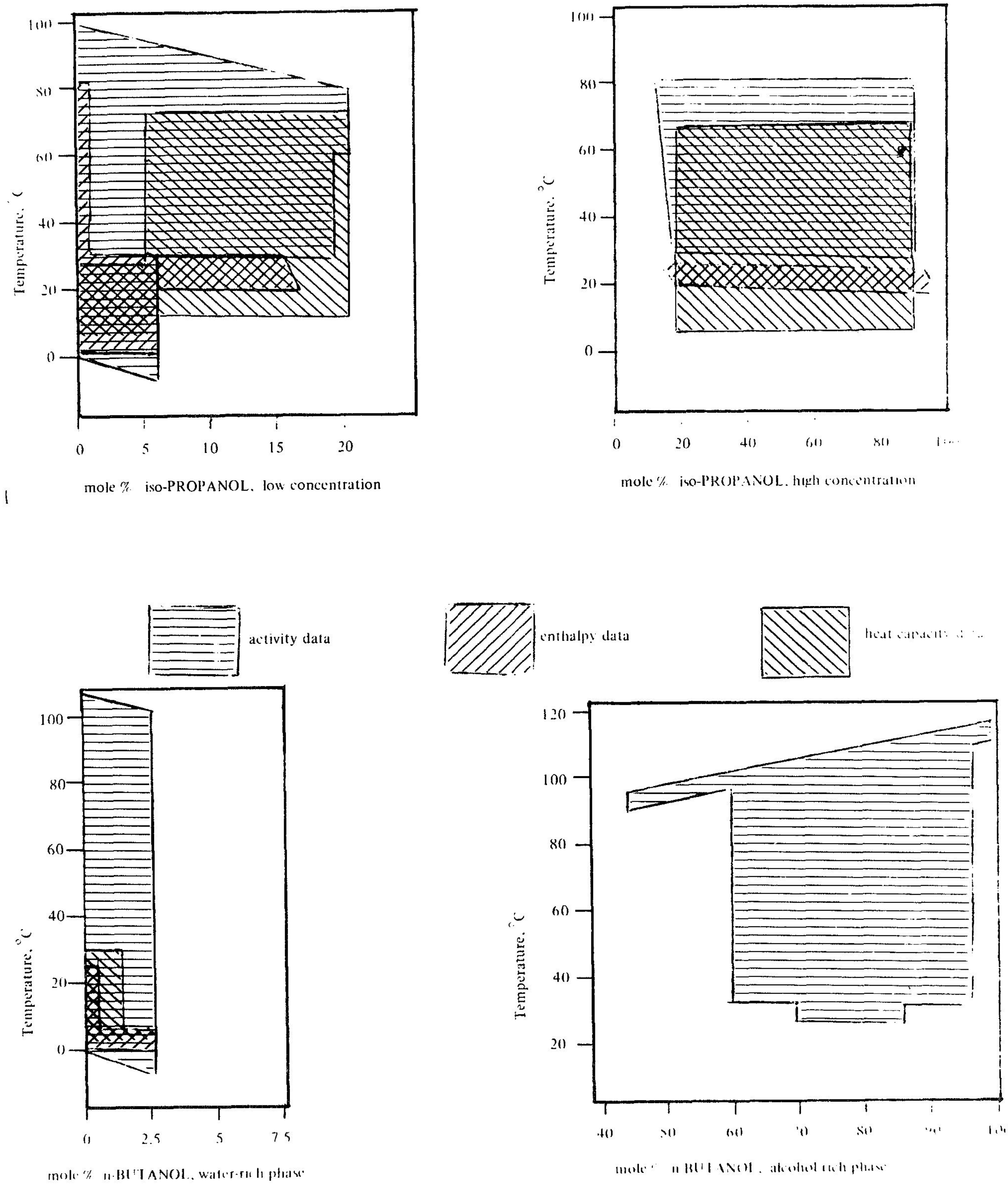

Figure 2. Temperature and Concentration Ranges of Experimental Data

Table 19

Auxiliary Data for the Pure Components

Temperature °C	P_1° mmHg*	C_p°, cal deg^{-1} mol^{-1}	$-\beta$, cm^3 mol^{-1}	P_2° mmHg*	C_p°, cal deg^{-1} mol^{-1}	$-\beta$, cm^3 mol^{-1}	P_2° mmHg*	C_p°, cal deg^{-1} mol^{-1}	$-\beta$, cm^3 mol^{-1}
	water			methanol			ethanol		
10	9.2	18.05		54.1	18.75		24.0	25.64	
15	12.8	18.02		72.3	18.96	2215	32.9	26.04	
20	17.5	18.00	1314	95.6	19.17	1980	44.6	26.46	3436
25	23.6	18.00	1194	125.0	19.39	1778	59.8	26.90	2981
30	31.8	17.99	1092	161.8	19.63	1603	79.2	27.36	2604
40	55.3	17.99	930	263.2	19.97	1320	135.0	28.36	2026
50	92.6	18.00	811	413.5	20.57	1102	221.6	29.46	1615
60	149.4	18.02	720	629.8	21.22	933	351.9	30.65	1318
70	233.8	18.04	651	932.4	21.92	801	542.2	31.93	1100
80	355.3	18.07	597			695	813.0	33.31	937
90	525.9	18.11	555				1189.3	34.78	813
100	760.0	18.15	522						717
	n-propanol			iso-propanol			n-butanol		
10		31.6	4078	17.1	34.1	3965		40.03	
15	10.5	32.3	3746	24.0	35.0	3556		40.77	
20	14.9	33.0	3415	33.1	35.8	3147		41.51	
25	20.9	33.7	3140	45.2	36.8	2828	6.2	42.31	3940
30	28.7	34.5	2894	60.8	37.6	2552	8.9	43.12	3670
40	52.4	36.1	2479	106.7	40.3	2105	17.8	45.05	3057
50	91.2	37.9	2143	179.5	42.5	1763	33.2	47.08	2617
60	152.2	39.8	1769	290.5	44.6	1497	59.0	49.18	2263
70	244.8	41.7	1643	456.0	46.3	1288	100.1	51.30	1974
80	380.7	43.6	1454	693.7	48.0	1122	162.9	53.45	1737
90	574.6		1296	1027.			255.8		1539
100	844.		1161				388.7		1373

*Constants in the Antoine Vapor Pressure Equation, $\log P = A - B/(C + t)$

	A	B	C
water, 0-30°C	8.184254	1791.3	238.1
water, 30-40°C	8.139399	1767.262	234.10
water, 40-50°C	8.088677	1739.351	234.10
water, 50-60°C	8.046420	1715.429	232.14
water, 60-70°C	8.011630	1695.167	230.41
water, 70-80°C	7.984559	1678.948	228.97
water, 80-90°C	7.963429	1665.924	227.77
water, 90-100°C	7.948396	1656.390	226.86
methanol, -14-65°C	7.89750	1474.08	229.13
methanol, 65-110°C	7.97328	1515.14	232.85
ethanol, -2-100°C	8.32109	1718.10	237.52
n-propanol, 2-120°C	7.84767	1499.21	204.64
iso-propanol, 0-101°C	8.11778	1580.92	219.61
n-butanol, 15-131°C	7.47680	1362.39	178.77

II. Bibliography

The bibliography on pages 34 to 80 lists references to numerical data on the thermodynamic properties of aqueous solutions of organic compounds of importance in biochemistry. It was compiled through a search of the world's scientific literature for the period 1895 to 1969. Properties considred include phase equilibrium data such as vapor pressure, vapor-liquid compositions, freezing point, boiling point, and solubility; calorimetric data such as heats of solution, dilution, and chemical reactions in solution and heat capacity; reversible cell potentials, acid and basic dissociation constants; and equilibrium constants of enzyme catalyzed reactions. Emphasis was placed on binary systems although some important ternary systems were included. We believe the list includes all significant data for simple organic compounds such as formaldehyde, acetaldehyde, acetone, C_1 - C_4 alcohols and mono- and dicarboxylic acids, certain hydroxy- and keto-acids, amino acids, sugars and related poyhydroxy alcohols, and urea. It is not complete for compounds of more complicated structure such as heterocyclic nitrogen compounds and their derivatives, nucleotides and nucleosides. Macromolecules are not included. A compound index is given on pages 81 to 90.

Note that several reference numbers have been skipped in the bibliography because the corresponding references were deleted from the list.

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Compound Index

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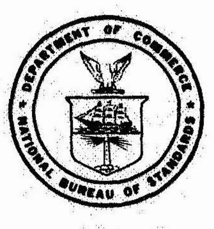

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