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Heats of mixing

Heats of Mixing: Measurement and Prediction by an Analytical Group Solution Model

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ENTHALPIES DE MELANGE: MESURES ET PREDICTIONS PAR UNE METHODE ANALYTIQUE DE CONTRIBUTIONS DE GROUPES

RESUME

Le modèle dit "de contributions de groupes" de Ratcliff et Chao pour la prédiction des chaleurs de mélange des solutions liquides a été mis sous une forme analytique en utilisant l'équation de Wilson. Ceci élimine certaines des restrictions et imprecisions du modèle précédent et le rend particulièrement adapté a la corrélation de données expérimentales et à la prédiction des chaleurs de mélange.

Un calorimètre isotherme semi-continu du type "Van Ness" permit des mesures précises et très rapides des chaleurs de mélange. L'ensemble des données ainsi obtenues a partir de plusieurs systèmes alcool/alcane, et à diverses températures, a pérmi d'abord de vérifier le modèle analytique, ensuite de déduire les paramètres de Wilson relatifs aux groupes methylene/hydroxyl, lorsque ces deux groupes sont utilisés conjointement dans un domaine de température allant de 15° a 55°C. A les températures semblables, il est alors possible de prédire, sans aucune autre mesure experimentale, les chaleurs de mélange de deux ou plusieurs constituants liquides ne contenant que ces deux groupes.

Un accord quantitatif entre la theorie et les experiences a été egalement obtenue pour les mélanges binaires constitués, d'une part de n-pentanol ou d'isopentanol, d'autre part d'isomeres de l'hexane. Pour ces systèmes, la ramification ne present qu'un effect d'ordre secondaire, qui ne demande ni traitement spécial, ni modification du modèle analytique.

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ABSTRACT

The Group Solution Model of Ratcliff and Chao for heats of mixing of liquid mixtures has been put in an analytical form using the Wilson equation. This procedure obviates some of the limitations and inaccuracies of the previous model and is very powerful for correlating and predicting heat of mixing data.

A semi-continuous isothermal calorimeter of the Van Ness type built during this work has allowed very rapid measurements of accurate heat of mixing data. This collection of data on several alcohol/alkane systems at different temperatures allowed a very good test of the analytical model. Group Wilson parameters were generated for methylene/hydroxyl mixtures from 15 to 55°C. At temperatures within or close to this range, these parameters allow the prediction of heats of mixing of binary or multicomponent mixtures containing these two groups; no experimental data are required.

Quantitative agreement between theory and experiment was also obtained for binary mixtures of n-pentanol or isopentanol with hexane isomers. Branching in these systems has only a second order effect and modification of the model to allow for branching is unnecessary.

HEATS OF MIXING:
MEASUREMENT AND PREDICTION BY AN ANALYTICAL GROUP SOLUTION MODEL

by

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INTRODUCTION

Information on heats of mixing of liquid solutions is important beyond its usefulness for heat effect calculations. Heat of mixing gives a direct measure of the rate of change of excess free energy with temperature. Excess free energy is basic to the study, correlation and prediction of vaporization properties of non-ideal solutions. Heat of mixing information, when available, provides a reliable means for extrapolation of such vaporization properties over a range of temperature.

Unfortunately, no generally satisfactory methods of prediction for highly non-ideal mixtures have been derived from rigorous liquid state theories. The analytical group solution model (AGSM) offers a method of wide applicability while requiring a minimum of experimental data. The model is perhaps simple but nonetheless isolates and takes account of the important effects.

The attractiveness of group solution models stems from the fact that large numbers of compounds are made up of relatively few groups. Once the group parameters are evaluated, mixture properties can be predicted for all mixtures that contain these groups. Complicated multicomponent mixtures can be handled as they are reduced to systems containing only a few groups. It entails the following:

1) A suitable reduction of experimentally obtained heats of mixing to obtain a set of parameters for each pair of structural groups in a specific system. These parameters are group parameters rather than molecular parameters.

2) The use of these parameters to predict properties of other systems which contain the structural groups.

The accuracy of such a model depends not only on the effective extrapolation involved and the inherent limitations of the approach, but also on the accuracy of the base data. Excellent experimental data over a reasonable range of temperature are required for a good test of the model. Literature data are restricted to a small temperature range. Therefore, experimental measurements are necessary.

A semi-continuous isothermal calorimeter of the Van Ness type built during this work has allowed very rapid collection of accurate heat of mixing data.

The calorimeter was essentially operated by mixing two components, each at the same constant temperature in a thermally insulated vessel with no vapor space at such a rate as to maintain the temperature of the solution in the vessel at a given temperature while adding energy to the solution electrically. Periodically, the mixing process was interrupted and heating was discontinued. The composition of the mixture in the vessel was then determined and the amount of energy added was recorded.

Thus, the objectives of the present work reflect both of the following practical aspects. The construction of a calorimeter for rapid and accurate measurements of heats of mixing. The data obtained from this apparatus are not only useful in themselves, but also serve as base data for developing a predictive model which would be simple, easily applicable and suitable for computer use. The present objectives emphasize an engineering approach rather than a theoretical one.

1. SOLUTION OF GROUPS APPROACHES

The "group solution" approach, also called "group interaction" approach, treats liquid mixtures in terms of their constituent functional groupings, e.g. CH_2, OH, CO.... This treatment is based on the intuitive assumption that the intermolecular forces can be considered to be of a local nature between adjacent groups and that the nature of a group is independent of how it is linked in a molecule. Interatomic forces are short range so that the effect of distant groups will be small. As there are many fewer groups than molecules, the group contribution methods have the advantage of predicting solution behavior from a minimum of experimental information.

As will be illustrated below, surprisingly far-reaching and precise estimates of properties in mixtures of simple organic molecules can be made on the basis of appropriate systematic observations and correlations with contributions from structural groupings.

1.1 Langmuir Model

The most significant early description of simple mixtures in terms of groups was probably given by Langmuir (L1) some fifty years ago. Langmuir began with the basic assumption that the force field around a group or radical which is accessible to other molecules is characteristic of that group or radical and is largely independent of the nature of the rest of the molecule. By summing the interfacial interaction energies between dissimilar groups, weighted according to the surface fractions of these groups in their respective molecules and according to the overall surface fraction of solute and solvent, Langmuir derived an expression for the partial pressures in a mixture of two components:

$$P_1 = P_1^{sat} x_1 \exp (s_1 \epsilon S_2^2/RT) \qquad (1.1)$$

where P_1 is the partial pressure of component 1, s_1 is the molecular area of component 1 and S_2 is the surface fraction of component 2. ϵ is an interfacial energy per unit area and is characteristic of the kinds of group and group fractions in the respective components 1 and 2. Langmuir dealt with molecules of the sort R-X in which a nonpolar R group is considered a single group and X is a polar group. Apparently Langmuir did not pursue the approach very far, perhaps as a result of inadequate experimental data.

1.2 Butler et al Model for Limiting Activity Coefficient

The work of Butler et al. (B1,B2) is basically a group approach. Butler considered the infinitely dilute solution of a series of solutes in a given solvent as the simplest case for study. He systematically measured Henry's law constants for a wide range of solutes within a given family of solutions and observed a simple relation between solute carbon number and its limiting activity coefficient. He also indicated that this relation depends roughly on the nature of the polar grouping.

1.3 Pierotti Correlations

Some ten years later, Pierotti et al. (P1,P2) at Shell Development Co. began a more extensive systematic study of homologous series. Here, as had Butler, they considered the infinitely dilute solution to be the least complicated and most promising for the study of group effects. The dilute regions are of considerable technological importance since applications are frequently in purifications. Moreover, in view of the usual shape of log γ - concentration curves, interpolations from dilute regions to the standard state can be expected to be more precise than extrapolations from data in the middle range of concentrations.

In practice, this work involved measuring γ's at high dilution for homologous series of solvents and inspecting the dependence of log γ^{o}'s upon the carbon numbers of solute and solvent. For n-alkyl homologs, a series of relations were developed for successively more complicated cases. The procedure can be thought of as simply determining the response of log Y^{o}'s as a function of the number of methylene (methyl) groups, n_1 and n_2, of the solute and solvent molecule for the case in which the groups are connected as in homologous series. Thus, for paraffin-paraffin mixtures, that s the series H $(CH_2)_{n1}$H in the series H $(CH_2)_{n2}$H, the deviations from ideality are relatively small. The expression for the congruent solutions of Brønsted and Koefoed (B1) was adopted as sufficiently precise, i.e.,

$$\log \gamma_1^{o} = D(n_1 - n_2)^2 \qquad (1.2)$$

where D is a constant.

For a homologous series of solutes of the type, H $(CH_2)_{n1}$ R_1, in a homologous series of solvents of the type H $(CH_2)_{n2}$ R_2, they found that:

$$\log \gamma_1^{o} = A_{12} + \frac{F_2}{n_2} + B_2\frac{n_1}{n_2} + \frac{C_1}{n_1} + D_o(n_1 - n_2)^2 \qquad (1.3)$$

where all the coefficients A_{12}, F_2, B_2, C_1 and D_o are temperature dependent and characterize the various group interactions.

Although the model was derived for the special case of solute at infinite dilution in solvent, the success with which very broad range of solute-solvent cases have been dealt with suggests that any environment, such as the range of finite concentrations in a binary or more complex mixtures, might be similarly treated.

There has been no systematic attempt to define Pierotti characterizations for molecular mixtures, but the viewing of a molecular environment as an environment of its constituent groups has proved a valuable guide in making estimates of activity coefficients in mixtures.

1.4 Group Interaction Model

Redlich, Derr and Pierotti (R1) later developed a group interaction model which calculates the heat of solution as the sum of contributions from interacting groups proportional to the number of groups present, a group cross section characteristic of each kind of group and an interaction energy characteristic of each group pair. As does the original Langmuir model, it neglects any local ordering or segregation except in so far as it is implicitly taken into account through the determination of the parameters from experimental data. It provides a relation for the partial molar free energies with concentrations expressed in surface fractions. As a result, the limiting partial molar free energies in a binary are in the ratio of the total molecular cross sections of the component molecules.

In a companion paper, Papadopoulos and Derr (P4) provided a preliminary test for this model for hydrocarbon systems. But as energy considerations are ignored in evaluating the probability of interactions, their model only applied to hydrocarbon mixtures in which the interaction energies are of comparable order of magnitude. For mixtures containing polar groups it is not possible to ignore preferential interactions due to large interaction energy differences between groups.

The group interaction theory of Redlich, Derr and Pierotti was further developed for heats of mixing by Chao and Coworkers (C1) to apply to solutions containing polar substances. Chao has considered the probability of interaction between two groups to be dependent both on the magnitude of the interaction energy between the groups and on the free surface area of the groups. The surface areas have been calculated from realistic geometric models of the molecules involved, i.e. from Van der Waal's and covalent radii of atoms. Local concentrations due to energy differences are taken into account using Boltzmann type relations. The interaction energies between group pairs in the mixtures have been determined as adjustable parameters in fitting the theory to experimental data. The model has provided satisfactory qualitative predictions for heats of mixing in n-alcohol/n-paraffin mixtures with reasonable values for the group interaction energies.

The relative success of Chao's model gives some credibility to the basic assumptions.

1.5 Solution of Groups

Wilson (W2) has proposed a solution of groups approach which estimates the partial molar excess free energies as the sum of group contributions and provides a concentration dependency for these group contributions. In this case, a "group" portion of the partial excess free energy is taken as the difference between contributions in solution and molecular standard state,

$$\log \gamma_i^G = \sum_k N_{ki} (\log \Gamma_k - \log \Gamma_{ki}^*) \qquad (1.4)$$

where log Γ's represent group contributions in the solution, the superscripts G and * denote the group contribution and the standard state respectively, and N_{ki} is the number of groups of type k in molecular species i.

Γ is taken as a function only of group fraction, temperature and pressure,

$$\Gamma_k = f_k(X_1, X_2 \ldots, T, P) \qquad (1.5)$$

where the X's are the group fractions:

$$X_k = \frac{\sum_i N_{ki}\, x_i}{\sum_i \sum_k N_{ki}\, x_i} \qquad (1.6)$$

The molar activity coefficient is taken as the sum of the group contribution and a contribution due to the relative sizes of the molecules:

$$\log \gamma_i = \log \gamma_i^G + \log \gamma_i^S \qquad (1.7)$$

where the size contribution, denoted by the superscript S, represents the only distinction between the environments of the same group constitution and different molecular constitution. It is evaluated from a Flory-Huggins type expression using only the number of groups in the respective molecules of the mixture:

$$\log \gamma_i^S = \log \frac{N_{ki}}{\sum_i N_{ki}\, x_i} + 0.4343\left(1 - \frac{N_{ki}}{\sum_i N_{ki}\, x_i}\right) \qquad (1.8)$$

Wilson and Deal applied such an approach to two fairly extreme cases - CH_2-OH and CH_2-CN mixtures - making no distinction between methylene and methyl groups. Substantial agreement was obtained over a wide range of values from a single base system; the logarithms of activity coefficients are generally estimated to within about 10%. For highly non-ideal systems, the size contribution is only a minor contribution compared to the group contribution. Therefore, the error in evaluating the size would be minimized.

As this model is applied to paraffin mixtures, Ratcliff and Chao (R1) found that the Flory-Huggins equation predicts values which are numerically too large. One may think that the size contribution has been overestimated. This conclusion leads to the modified group solution model of Ratcliff and Chao (R1), with another expression for log γ_i^S using Bronsted and Koefoed's equation (B3):

$$\log \gamma_1^S = B(N_{k1} - N_{k2})^2 x_2^2 \qquad (1.9)$$

where B is a temperature dependent constant. For multicomponent mixtures,

$$\log \gamma_i^S = B(N_{ki} - \sum_j x_j N_{kj})^2 \qquad (1.10)$$

Tests of this model on various alcohol/alkane and alcohol/water systems are quite successful. Maripuri and Ratcliff later applied the model to alkane/ketone systems (M1) and to mixtures containing aromatic hydrocarbons (M2).

1.6 Analytical Solution of Groups

A new step in the group contribution approach was made by Deal and Derr recently (D1) by using an analytical expression for the group activity coefficient Γ. They have chosen to represent the log Γ - concentration dependency with the Wilson (W1) molecular free energy expression based largely on the observation that this relation gives a more suitable shape to log Γ_k - concentration dependencies in binary systems. The use of the Wilson equation also permits the treatment of binary and multicomponent systems having many kinds of groups and makes computer calculation possible.

The form of Wilson equation in representing the group activity coefficient is shown in the following equation:

$$\log \Gamma_k = - \log \sum_{l=1}^{N} X_l a_{kl} + 0.434\left(1 - \sum_{l=1}^{N} \frac{X_l a_{lk}}{\sum\limits_{m=1} X_m a_{lm}}\right) \qquad (1.11)$$

where the a's are binary group parameters.

The development is particularly attractive for correlating complex systems which contain more kinds of molecules than kinds of groups, since many fewer adjustable parameters are required. Such an "analytical solution of groups model" has the advantage of storing an enormous amount of data using only a few temperature dependent parameters. The advantages of the analytical model will be discussed in detail later.

Some similar but more theoretical approaches suggest that further work in theories of mixtures using a group interaction approach will result in quantitative predictions of solution behavior. Three recent papers published by Chao and coworkers (C2-4) show interesting results in this direction. Statistical thermodynamics based on cell theory and quasi-lattice theory has been developed for pure n-alkane and n-alcohol molecules and their mixtures. Formulas for the excess properties have been derived from the partition function and applied to n-alcohol/n-alkane and n-alcohol/n-alcohol mixtures. Predictions of heats of mixing are within about 10% on alcohol/alkane mixtures. The deviation tends to become larger for the lower alcohol solutions. The solution behavior of alcohol/alcohol mixtures appeared not to be well described by the group interaction model.

As will be apparent, this "solution of groups" approach of treating mixtures in terms of their constituent groupings is thermodynamically sound. The projections of the model are particularly valuable in process designs when no experimental data are available.

Nomenclature

a_{ij}	group Wilson parameter in equation (1.11)
N_{ki}	number of groups of type k in molecular species i
P	pressure
R	ideal gas constant
s	molecular area in equation (1.1)
S	surface fraction in equation (1.1)
T	absolute temperature
x	mole fraction
X	group fraction

Greek Letters

γ	liquid phase activity coefficient
ϵ_{8}	energy constant in equation (1.1)
Γ	group activity coefficient

Subscripts

i	molecular species i
k	group species k

Superscripts

G	group contribution
S	size contribution
*	standard state

2. GROUP SOLUTION MODEL FOR HEATS OF MIXING

2.1 Description of the Model

The group solution model of Ratcliff and Chao has been used previously to predict excess free energies (R2-3, M1-2) and transport properties (R4) of non-ideal systems. The application of a similar model has been extended to excess enthalpies of mixing (N1-2).

With the idea that a group is any convenient structural unit such as $-CH_2-$, OH- ...., the present model rests on the following four postulates:

Postulate 1

The non-ideal behavior of a molecule in a liquid solution may be broken down into two independent parts. One is associated with the overall size of the molecule and the other with the interactions between the functional groups of the molecule and those present in the solution.

This first postulate may be written in terms of heats of mixing as:

$$\Delta H = \Delta H^G + \Delta H^S \tag{2.1}$$

where the superscripts S and G denote the size and group contributions respectively.

Postulate 2

The size contribution accounts only for the differences in size of the molecules, and can be obtained from the heats of mixing of n-alkane mixtures.

Postulate 3

The group contribution to ΔH is assumed to be the sum of the individual contributions of each group present, i.e., all groups are assumed to act independently. Each group is imagined as an individual entity in a "solution of groups", and a group excess enthalpy H_k of a group k is defined in a similar manner to a molecular excess enthalpy. By definition, H_k is zero for a solution containing only group k. We thus have the relation:

$$\Delta H^G = \sum_i x_i \overline{\Delta H_i^G} \qquad (2.2)$$

and

$$\overline{\Delta H_i^G} = \sum_k N_{ki}(H_k - H_{ki}^*) . \qquad (2.3)$$

where N_{ki} = number of groups of type k in molecular species i

H_{ki}^* = excess enthalpy of group k at standard state.

The standard state chosen for a group is that of the pure molecular species i under consideration. This agrees with normal practice, and assures that the partial molar heats of mixing are zero for pure compounds. The same group must be referred to different standard states depending on the molecular species under consideration. The choice of the groups is arbitrary, but consistent definitions must be employed both in the determination of H_k and in the application of the model to new systems.

Postulate 4

At a given temperature and pressure, the group excess enthalpies H_k are functions only of the group composition, and therefore are independent of the molecular species under consideration.

$$H_k = f_k(X_1, X_2, \ldots X_k, T, P) \tag{2.4}$$

The group fraction X_k is computed in the same way as a mole fraction, i.e.,

$$X_k = \frac{\sum_i x_i N_{ki}}{\sum_i \sum_k x_i N_{ki}} \tag{2.5}$$

2.2 Limitations of the Model

2.2.1 Limitations Inherent in the Model

The model takes into account the differences in molecular size, but not molecular shape. The model predicts the same heats of mixing for isomeric molecules in solutions of identical group composition. This restriction is not very serious and will be discussed in the last chapter on the study of mixtures of alcohol with hexane isomers. Since only highly non-ideal systems are considered, even approximate predictions are valuable from a practical point of view.

Another assumption inherent in the model is that the forces acting on a group are functions only of the average group concentration. No account is taken of the tendency of the molecule to segregate. However, as predictions for new systems are made through group excess enthalpies computed from experimental data on chosen reference systems containing the same groups, some cancellation of errors would be expected when applying the data from one mixture to another.

2.2.2 Limitations in the Application of the Model

In the earlier use of the model (NI-2), experimental heats of mixing for reference systems were used to compute H_k's. These were being expressed as functions of group composition, either graphically or by fitted power series. This computation procedure resulted in the following limitations or inaccuracies:

1) The number of groups present in the reference system can not exceed the number of molecular components, since otherwise equation (2.3) will provide insufficient equations to solve for the H's.

2) Unless each molecular species consists of a single group, it is impossible to compute all the H's directly from the experimental data for a single reference system. For example, if for mixtures of the groups methylene and hydroxyl, we chose n-butanol/n-hexane as the reference system, then we can only compute H_{CH_2} and $(H_{OH} - H^*_{OH,butanol})$ from equation (2.3). We can nevertheless now predict heats of mixing of any mixture as long as the individual molecular constituents lie within the group compositions represented by pure butanol, i.e. $X_{CH_2} = 0.80$, and pure hexane, i.e. $X_{CH_2} = 1.0$. In the particular example, the methylene group fractions range from 0.80 to 1.0 and the model can be used to predict heats of mixing for pentanol/alkane systems $(0.833 < X_{CH_2} < 1.0)$ but can not be applied to propanol/alkane systems $(0.75 < X_{CH_2} < 1.0)$ without uncertain extrapolation.

However, if we wish to extend predictions to lower CH_2 concentrations, we are forced to choose a second reference system covering this extended range. Furthermore, we need data for both systems at the same temperature, pressure and preferably an appreciable overlap in group composition.

3) On the previous model, H_k's were expressed as functions of group composition by fitted power series with arbitrary parameters. These parameters could be used only at the studied temperature. Interpolation or extrapolation of temperature in making the predictions can be inaccurate.

The application of this model has been investigated for systems containing aliphatic alkanes and alcohols (N3) at 25°C and 45°C. For 14 binary group mixtures, the model required experimental data for two reference systems; one to evaluate the size contributions and the other, the group contributions. The model gave very satisfactory predictions of heats of mixing with an average root-mean-square deviation of about 11% over a group CH_2 composition range from 0.80 to 1.0.

The size contribution to heats of mixing was very small compared to the group contribution in the 14 systems studied. Neglect of the size contribution did not significantly decrease the prediction accuracy (N2). Derr and Deal (D1) have suggested that the size term could be neglected in developing a group model for heats of mixing since this term can be accounted for by entropy. Although we expect that for mixtures of component molecules with large differences in size, the effect might be of some significance, e.g. propanol/n-hexadecane; this neglect added the advantage that predictions are not limited by the lack of heat of mixing data for low molecular weight alkanes in computing the size contribution.

Nomenclature

H_k	excess enthalpy of group k
N_{ki}	number of groups of type k in molecular species i
P	pressure
T	absolute temperature
x	mole fraction
X	group fraction
ΔH	heat of mixing (excess enthalpy) per mole of mixture
$\overline{\Delta H}$	partial molar excess enthalpy

Subscripts

i	molecular species i
k	groups species k

Superscripts

G	group contribution
S	size contribution
*	standard state

3. THE ANALYTICAL GROUP SOLUTION MODEL

All the limitations in the applications of the group solution model can be eliminated by the application of an analytical group solution model. This involves the choice of a suitable analytical function for f_k's of equation (2.4). The function should have a minimum of adjustable parameters and should represent the data with minimal loss of accuracy. If such a function can be found, it would also reduce the data required, and be readily amenable to computer calculations and to temperature interpolations.

3.1 Analytical Expression for Molecular Activity Coefficient

Wilson (Wl) derived a semi-empirical equation for the excess free energy ΔG^E from a theoretical expression for ΔS^E. Flory and Huggins (Fl) had shown that for a binary athermal mixture (i.e. a mixture where $\Delta H^E = 0$), the excess Gibbs free energy for a binary mixture resulting from molecular size difference is given by:

$$\frac{\Delta G^E}{RT} = x_1 \ln \frac{\Phi_1}{x_1} + x_2 \ln \frac{\Phi_2}{x_2} \tag{3.1}$$

where Φ_i = volume fraction of component i, that is,

$$\Phi_i = \frac{x_i\ v_i}{\sum_i x_i\ v_i} \qquad (3.2)$$

v_i is the molar volume of pure liquid i.

Wilson suggested that in a real (i.e. not athermal) solution, equation (3.1) could be used for ΔG^E provided that the overall volume fractions Φ_1 and Φ_2 be replaced by local volume fractions ξ_1 and ξ_2. Wilson's suggestion produces an equation highly useful for strongly non-ideal binary and multicomponent mixtures.

To understand the significance of local volume fractions, we first explain what we mean by local mole fractions. Molecules 1 and 2 in a binary liquid mixture do not, in general, distribute themselves in a random manner but tend to segregate, depending on what attractive forces are larger: 1-1, 2-2, or 1-2.

To illustrate this idea, Figure (3.1) shows schematically a mixture of 20 shaded molecules and 20 unshaded molecules. The overall mole fraction is therefore 0.5 for both components.

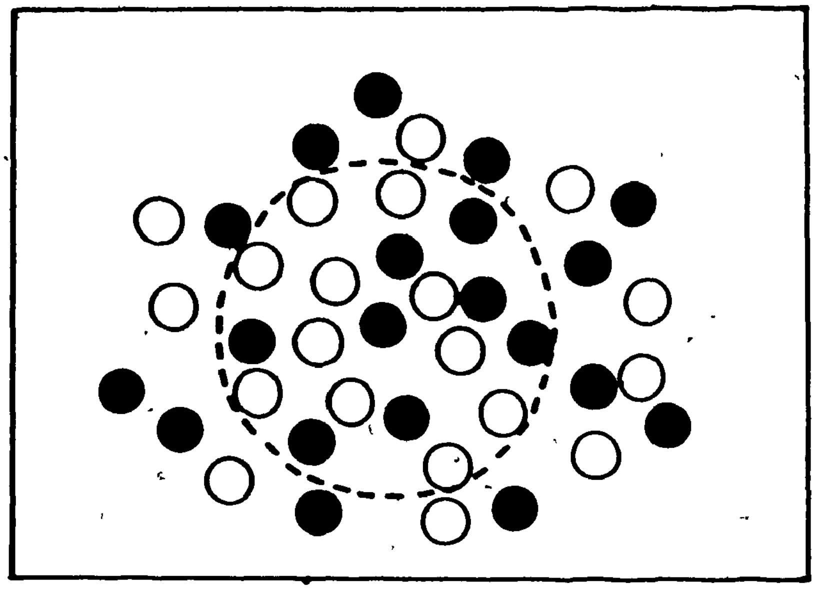


FIGURE 3.1: Local Composition

However, if attention is fixed on the intermediate surroundings of a central shaded molecule (area within the circle) we find that the local mole fraction of shaded molecules is 8/19.

In a binary mixture, there are four local mole fractions but only two of these are independent. The symbol x_{ij} stands for the local mole fraction of molecule i around a central molecule j. Thus in a binary mixture we have:

$$x_{12} + x_{22} = 1 \tag{3.3}$$

$$x_{21} + x_{11} = 1 \tag{3.4}$$

To relate local mole fractions to overall mole fractions we assume a relation of the Boltzmann type:

$$\frac{x_{21}}{x_{11}} = \frac{x_2 \exp(-g_{21}/RT)}{x_1 \exp(-g_{11}/RT)} \qquad (3.5)$$

where g_{21} is an energy term reflecting the forces between molecules of species 1 and 2 and g_{11} is a similar term for forces between molecules of species 1.

Also we have:

$$\frac{x_{12}}{x_{22}} = \frac{x_1 \exp(-g_{12}/RT)}{x_2 \exp(-g_{22}/RT)} \qquad (3.6)$$

and

$$g_{12} = g_{21}$$

The local volume fractions are given by weighted local mole fractions, the weighting factors are set equal to the pure component molar volumes v_i,

$$\frac{\xi_{21}}{\xi_{11}} = \frac{v_2 \, x_{21}}{v_1 \, x_{11}} \qquad (3.7)$$

and

$$\frac{\xi_{12}}{\xi_{22}} = \frac{v_1 \, x_{12}}{v_2 \, x_{22}} \qquad (3.8)$$

where $\xi_{21} = 1 - \xi_{11}$

and $\xi_{12} = 1 - \xi_{22}$ (3.9)

Substituting equations (3.5), (3.6) and (3.9) to equations (3.7-8) we arrive at the following expressions for local volume fractions ξ_{11} and ξ_{22},

$$\xi_{11} = \frac{x_1}{x_1 + x_2(v_2/v_1)\exp(-(g_{21}-g_{11})/RT)} \qquad (3.10a)$$

and

$$\xi_{22} = \frac{x_2}{x_2 + x_1(v_1/v_2)\exp(-(g_{12}-g_{22})/RT)} \; . \qquad (3.10b)$$

Now, upon substitution ξ_{11} for Φ_1 and ξ_{22} for Φ_2 in equation (3.1), we obtain;

$$\Delta G^E/RT = -\sum_i x_i \ln\left(\sum_j x_j A_{ij}\right) \qquad (3.11)$$

where A_{ij} is given by:

$$A_{ij} = (v_j/v_i)\exp(-(g_{ij} - g_{ii})/RT) \qquad (3.12)$$

For binary mixtures, equation (3.11) becomes

$$\Delta G^E/RT = -x_1 \ln(x_1 + A_{12}x_2) - x_2 \ln(x_2 + A_{21}x_1) \qquad (3.13)$$

From equation (3.13), the activity coefficients of the two components are determined by:

$$\ln \gamma_1 = -\ln(x_1 + x_2A_{12}) + 1 - \frac{x_1}{x_1 + x_2A_{12}} - \frac{x_2A_{21}}{x_2 + x_1A_{21}} \tag{3.14a}$$

$$\ln \gamma_2 = -\ln(x_2 + x_1A_{21}) + 1 - \frac{x_2}{x_2 + x_1A_{21}} - \frac{x_1A_{12}}{x_1 + x_2A_{12}} \tag{3.14b}$$

where A_{12} does not equal A_{21} although g_{12} does equal g_{21}.

Wilson's treatment is particularly successful for mixtures containing alcohols in non-polar solvents. One of the main advantages of Wilson's equations follows from its straightforward extension to multicomponent mixtures. The important feature of these equations is that all parameters A_{ij} may be obtained from reduction of binary data; no ternary (or higher) constants are required.

3.2 Analytical Expressions for Group Activity Coefficients

Recently, Deal and Derr (D1) have chosen to represent the ln Γ concentration dependency by the Wilson molecular free energy expression, based largely on the observation that this relation gives a more suitable shape to the log Γ versus concentration curve in binary group systems.

The form of the Wilson equation in representing group activity coefficients is shown in the following equation, for a group k in a mixture containing groups $1 \ldots N$:

$$\ln \Gamma_k = -\ln \sum_{l=1}^{N} X_l a_{kl} + 1 - \sum_{l=1}^{N} \frac{X_l a_{lk}}{\sum_{m=1} X_m a_{lm}} \qquad (3.15)$$

where the a's are binary "group" parameters analogous to the conventional molecular binary parameters; the sums are to be taken over all groups in the mixture including k with $a_{kk} = a_{ll} = a_{mm} = 1$ and the X's are group fractions as defined by equation (2.5).

For the case of a solution containing only two groups 1 and 2, equation (3.15) takes the simple form:

$$\ln \Gamma_1 = -\ln(X_1 + X_2 a_{12}) + 1 - \frac{X_1}{X_1+X_2 a_{12}} - \frac{X_2 a_{21}}{X_2+X_1 a_{21}} \qquad (3.16a)$$

$$\ln \Gamma_2 = -\ln(X_2 + X_1 a_{21}) + 1 - \frac{X_2}{X_2+X_1 a_{21}} - \frac{X_1 a_{12}}{X_1+X_2 a_{12}} \qquad (3.16b)$$

The group solution model of Ratcliff and Chao for the excess free energies of liquid mixtures has also been put in analytical form using the Wilson equation. It was tested and found satisfactory for a wide range of mixtures containing the groups methylene and hydroxyl (R3).

3.3 Analytical Group Solution Model for Heats of Mixing

It seems possible now that independent correlations of heats of mixing by an analytical group solution model can be developed and would give a basis for projecting heats of mixing and temperature effects.

With the assumption of negligible size contributions, the analytical model for heats of mixing can be summarized by the following equations,

$$\Delta H = \Delta H^G = \sum_i x_i \overline{\Delta H_i^G} \tag{3.17}$$

$$\overline{\Delta H_i^G} = \sum_k N_{ki} (H_k - H^*_{ki}) \tag{3.18}$$

From the Gibbs-Helmholtz relation,

$$\frac{\partial}{\partial T} (\Delta G^E/RT)_{P,X} = - \frac{1}{RT^2} \Delta H \tag{3.19a}$$

H_k is related to Γ_k by:

$$\frac{\partial}{\partial T} (\ln \Gamma_k)_{P,X} = - (1/RT^2) H_k \tag{3.19b}$$

Thus by differentiating equation (3.16) with respect to temperature and rearranging the terms, the analytical expressions for H_k of binary group mixtures are given by:

$$H_1/RT^2 = X_2^2\, a_{12}\, b_{12}/(X_1 + X_2\, a_{12})^2 + X_2^2\, b_{21}/(X_2 + X_1 a_{21})^2 \tag{3.20a}$$

$$H_2/RT^2 = X_1^2\, a_{21}\, b_{21}/(X_2 + X_1 a_{21})^2 + X_1^2\, b_{12}/(X_1 + X_2 a_{12})^2 \tag{3.20b}$$

where $$b_{12} = \frac{\partial}{\partial T}(a_{12}) \quad \text{and} \quad b_{21} = \frac{\partial}{\partial T}(a_{21}) \tag{3.21}$$

The parameters (a's and b's) can be determined from experimental data for reference systems. To fix these parameters with confidence, we require data of high quality and quantity over a reasonable range of temperature. Recently, excellent heat of mixing data on n-alcohol/n-alkane mixtures have become increasingly available in the literature. However, the temperature ranges of these data are very restricted, e.g. 25°C-45°C (S1-3). Therefore, an isothermal semi-continuous calorimeter was built in order to extend this temperature range. Experimental measurements have been performed on several aliphatic alcohol/alkane mixtures at 15°C and 55°C and on branched pentanol/hexane systems at 25°C.

Nomenclature

A_{ij}	molecular Wilson parameter in equation (3.11)
a_{ij}	group Wilson parameter in equation (3.15)
b_{ij}	group Wilson parameter in equation (3.21)
g_{ij}	energy term in equation (3.5)
H_k	excess enthalpy of group k
N_{ki}	number of groups k in molecular species i
P	pressure
R	ideal gas constant
T	absolute temperature
v	molar volume of pure component
x	mole fraction
X	group fraction
ΔH	heat of mixing per mole of mixture
$\overline{\Delta H}$	partial molar heat of mixing
ΔG^E	excess free energy of mixing

Greek Letters

γ	liquid phase activity coefficient
Γ	group activity coefficient
Φ	volume fraction
ξ	local volume fraction

Subscripts

i,j	molecular species i,j
k	group species k

Superscripts

G	group contribution
S	size contribution
*	standard state
E	excess property

4. APPARATUS AND EXPERIMENTAL PROCEDURE

The importance of obtaining accurate enthalpy of mixing data has led to many diverse methods of measurement. The major differences between different calorimeters are the rapidity and the ease with which the data may be gathered.

Calorimeters may be classified according to their principle of operation: point-wise or semi-continuous. Point-wise isothermal calorimeters employed for the measurement of endothermic binary heats of mixing usually consist of a cell containing two liquids separated by some type of diaphragm or mercury trap. When the diaphragm is ruptured, the liquids mix and isothermal conditions are maintained by the addition of a measured quantity of electrical energy. Although, some investigators (A1),(B4),(M3) have obtained satisfactory measurements with calorimeters of this type, the basic principle limits the usefulness of such an apparatus: direct measurement of heats of mixing cannot be obtained below a certain concentration and many independent experiments are necessary for the measurement of the heat of mixing over the entire composition range, i.e., the procedure is very time consuming.

Semi-continuous isothermal calorimeters are based upon semi-continuous addition of one component into a cell initially containing the second component. The entire heat-of-mixing curve can be obtained by two experimental runs. Therefore, the procedure is rapid.

A semi-continuous isothermal calorimeter of the type built during this work was first described by Mrazeck and Van Ness (M4) in 1961. Subsequent refinement of this calorimeter by Van Ness and Coworkers (S2-3) has led to the development of a highly versatile instrument which lends itself to a rapid and routine production of data. There are, of course, many differences in detail such as will be found in any custom-built instrument.

The principle operation of this isothermal calorimeter is as follows: two liquids are mixed at constant temperature and pressure in an isothermally insulated vessel. Since all systems studied in this work are endothermic, the mixing process is accompanied by absorption of heat. Immediately upon mixing, the temperature of the system is maintained by adding electrical energy to the system. The amount of energy added is a measure of the heat of mixing.

An important feature of this calorimeter is the absence of vapor space. As pointed out by Mrazek and Van Ness (M4), this feature eliminates the source of error due to vaporization-condensation effects.

The calorimeter is shown in Figures (4.1-5).

4.1 Description of the Calorimeter

4.1.1 Calorimeter Housing

The calorimeter housing consists of a strip-silvered precision-bore, 150 ml Dewar flask. The Dewar flask was made up from precision-bore tubing with inside diameter of 1.999 ± 0.001" (H.S. Martin Co.). The use of the precision-bore glass tubing allows a concentric fit between the flask and the Teflon calorimeter plug.

4.1.2 Calorimeter Plug

The Teflon plug (Figure 4.3-4) is approximately 1" thick and is 1.978" ± 0.001" in diameter at room temperature of about 25°C. Sealing of the plug to the Dewar flask is accomplished by two Viton-A "O" rings (linear number 11-131, 11-132 or 11-133). The grooves are approximately 0.01" wide with a groove depth of 0.08". A tight seal is obtained at room temperature when the plug is positioned within the Dewar flask.

Four holes are bored through the plug. One hole contains four electric probes which are connected to the calorimeter heater. The second hole allows a glass-coated thermistor probe and its housing to pass through the plug. A threaded vent hole is also located in the calorimeter plug, when the screw is tightened, the calorimeter plug is sealed with the help of an "O" ring (linear number 11-009). The feed tube passes through the fourth hole which contains a hypodermic needle.

4.1.3 Calorimeter Heater

The calorimeter heater is a single filament, 0.00225" diameter Karma wire (an 80% nickel, 20% chrome alloy with addition of Al and Fe) having a resistance of about 45 Ohms, The heating element is non-conductively threaded on a small Teflon tube which then is mounted in a thin-wall copper housing tube. The ends of the heating filament are soldered to the heater probes with resin-core solder.

4.1.4 Calorimeter Stirrer-Baffle System

Mixing of the contents of the calorimeter is accomplished by a small Teflon-coated stirring bar. Four baffles are used to create an efficient circulation pattern. The baffle-magnet mixing system is supported by baffle rods screwed into the bottom of the calorimeter plug. The baffles and rods are constructed from coin silver. A large Alnico bar magnet is located outside the Dewar flask, in the constant temperature bath and activates the small magnet contained within the calorimeter. The external driving magnet is driven by a motor.

4.1.5 Calorimeter Mercury Trap

The calorimeter feed cup is supported by a Teflon strip fastened to the baffle rods. The end of the feed tube is drawn into the hypodermic needle which is centrally located in the Teflon cup. Mercury in the cup separates the liquid in the Dewar flask from that in the feed tube and feed bulb. Injected material flows upward into the system between the feed tube and mercury. A film type of flow is obtained. No mercury is discharged into the Dewar flask at both low and high rates of injection.

4.1.6 Feed System

The feed material is stored in a glass bulb C (Figure 4.1) having a capacity over 100 ml. This bulb is rested on a Plexiglass platform connected to the calorimeter support rack and is joined to the calorimeter feed tube by "0" ring pyrex joint. The feed bulb is also connected to a 5 ml water-jacketed, gravity filling automatic burette A

(Figure 4.1) and are held to proper alignment by clamps to a support stand above the constant temperature bath.

4.1.7 Calorimeter Electrical Circuit

All the systems studied are highly endothermic. Therefore, in order to maintain isothermal conditions on mixing, electrical energy is supplied to the calorimeter. The calorimeter circuits are shown in Figure 4.5. There are two fundamental measurements: energy input to the calorimeter and temperature of the solution in the Dewar flask.

4.1.7.1 Input Energy to the Heater

Three measurements are needed for this determination: current, potential drop across the heater and the length of time that current is flowing through the calorimeter heater.

4.1.7.2 Temperature of the Solution in the Dewar Flask

The temperature of the solution in the Dewar flask is sensed with a thermistor probe (Fenwal Catalog No. GA51P8). The resistance of such a probe is strongly temperature dependent and is measured by a guarded Wheatstone Bridge (Leeds and Northup, Model No. 4736). A Leeds and Northup Type 9834 D.C. null detector is used to sense the output of the Wheatstone bridge. The current flowing through the Wheatstone bridge circuit is supplied by a D.C. power supply (Hewlett Packard Model No. 6201B). It has been found that a voltage of less than 0.5 volt supplied to the bridge results in a self heating of the thermistor probe of less than 0.001°C. Note that the thermistor probe is periodically calibrated against a Leeds and Northrup Model 8164 Platinum resistance thermometer in a Mueller bridge circuit (Rubicon Co., Model 1550). The absolute accuracy of the temperature measurement is believed to be better than ±0.005°C.

The calorimeter heater circuit has been designed so that the power drawn from a power supply (Hewlett Packard Model No. 6201B) is constant whether the heater is on or off. This stabilizes the power source. Switching off the power between the ballast circuit and the calorimeter heater is performed with a 4PDT relay (Potter and Brumfield 4PDT relay, type GF17A, 120 VAC coil).

The ballast circuit is a 100 Ohm wire-wound potentiometer in series with a decade resistor box (Leeds and Northrup, Model No. 4776). They are used as a fixed resistor and are connected to a normally-closed position on the relay.

Two precision wire-wound resistor~~s (Leeds~~ and Northrup, No. SR-300-M-.01-A-1-DC and No. SR-2700-M-0.01-A-1-DC) in series form a voltage divider and are connected in parallel with the calorimeter heater. When the calorimeter is operating, the potential drop across the heater is given by a fraction of (300+2700)/300 = 10.000 by a D.C. digital voltmeter (Hewlett Packard Model No. 2401C).

A calibrated standard resistor of 1.00002 Ohms (Electro Scientific Industries, U.S.A., No. 743016) and a D.C. milliammeter (0-200 milliamperes) is used in setting the ballast resistor equal to the resistance of the heater circuit. If the ballast resistor is properly adjusted, the voltage across the standard resistor will remain constant as the heater circuit is switched to the ballast circuit.

A precision stopwatch (Canlab No. C6550) is connected to the normally-open position on the relay. The stopwatch and the heater are switched on or off by the 4PDT relay.

4.1.8 Constant Temperature Bath

The calorimeter must be immersed in a constant temperature environment in order to prevent heat transfer through the walls of the mixing Dewar flask and in order to insure that the injected component is at the same temperature as the solution into which it is injected.

A Tamson constant temperature bath (Neslab Instrument Inc. Model TEV45) provides a generous working area for such a purpose. Stirring of the water in the bath is performed by a circulation pump which also circulates the water from the bath to the water jacket of the automatic burette mounted above the bath. The setting temperature of the bath can be controlled to within ±0.005°C by the use of a fused quartz infra-red heater and a fast solid state relay. When the bath is operating at temperature below 40°C, circulation of cooling fluid through a cooling coil in the bath is recommended. This is accomplished by the use of a bath cooler (Neslab Instrument Inc. Model PCB-4) in combination with a circulating bath (Neslab Instrument Inc., Model TC9). This unit provides temperature-controlled water circulating through the cooling coil of the main bath.

The temperature of the thermostat bath is sensed with a quartz thermometer probe (Hewlett Packard, Model 2801A) which is periodically calibrated against a Platinum resistance thermometer (Leeds and Northrup Model 8164) in a Mueller bridge circuit already mentioned.

4.2 Operating Procedure

The experimental procedure for measuring the heats of mixing of binary systems is as follows (letters in parenthesis refer to Figure 4.1):

1) Constant temperature bath (F) is set at the desired temperature which is maintained to within ±0.005°C. The cooling fluid is used when the bath is operating at temperatures of 40°C and below.

2) The water in the bath is allowed to circulate to the water jacket of the burette (A). The burette is filled with one of the component of the binary mixture prior to the experiment.

3) The "0" rings are placed on the fixed Teflon plug (E) and the feed bulb (C) is connected to the feed needle (H) by a glass tubing carrying stopcock 2.

4) The small Teflon cup (G) is filled to within 1/16" of the top with mercury and the liquid in the bulb (C) is allowed to flow out of the needle (H) for several drops by opening connector stopcocks 1 and 2. Excess liquid is wiped away. A small droplet is allowed to collect at the needle. In one motion, touch the drop with the tip of a kleenex and slip the mercury cup over the needle allowing no air bubble to be trapped. The mercury level is then raised to mark M in the feed tube by opening stopcock 2 (stopcock 1 being closed) to the vacuum line attached above.

5) If bubbles form in the glass tubing, step (4) is repeated.

6) A 100 ml stoppered volumetric flask containing the second component is weigh-ed with a type B-6 Mettler balance. Approproximately 90 ml are poured into the Dewar flask (D) which is mounted on a platform below the calorimeter plug (E). The volumetric flask is immediately sealed and the Dewar flask

is quickly raised by a driving mechanism until the "O" rings surrounding the calorimeter plug are engaged. The volumetric flask is weighted again later with the Mettler balance.

7) Sealing of the calorimeter plug is completed. Vapor is driven out of the calorimeter by raising the Dewar flask. When the liquid is visible at the bottom of the vent hole, the Teflon vent screw is fastened under the calorimeter plug.

8) The calorimeter is placed into the constant temperature bath. The upper arm of the feed storage bulb is connected to the microburette (A). All stopcocks are slightly opened to see if the mercury level in the feed tube rises above or falls below the reference mark (M). If the mercury level begins to fall, the pressure in the lower part of the system is increased by raising the Dewar flask. If the mercury level tends to rise above the mark (M), this pressure is reduced by lowering the Dewar flask.

After several pressure adjustments, all stopcocks are fully opened and the mercury level in the feed tube is again set at the reference mark (M).

9) The electrical circuit is completed by connecting the calorimeter multi-contact electrical connector to a receptacle on the circuit control box.

10) The D.C. power supply is turned on and the ballast circuit is energised by closing a switch on the circuit.

11) The calorimeter stirrer is started and set at 200 RPM.

12) Decades on the Wheatstone bridge are set at a resistance corresponding to the bath set temperature. The voltage supply to the Wheatstone bridge is set at 0.4 volt. Since the calorimeter is not yet at the bath set temperature, the bridge is unbalanced. The unbalanced signal, properly attenuated, is indicated by a null detector in the bridge circuit.

13) The calorimeter is brought to thermal equilibrium with the constant temperature bath. Initially, the calorimeter is below the set temperature. Therefore the calorimeter heater is energized by closing a switch on the circuit. Energy is added to the calorimeter until the null detector indicates the Wheatstone bridge is balanced. When the bridge remains balanced at the same setting for 1/2 hour, it is assumed that the calorimeter and the bath are in thermal equilibrium.

14) The calorimeter is operated as follows:

14a. Timer is set at zero

14b. Mercury level in the feed tube is checked and adjusted if necessary so that the level corresponds to the reference mark (M)

14c. The initial reading of the burette is recorded. The first component in the burette is introduced into the Dewar flask by a drive mechanism. As the flask comes down, the liquid in the burette is drawn into the flask.

14d. The heater is turned on. The injection of the first component is introduced at a rate such that the temperature of the liquid in the flask is maintained to within 0.003°C of the set temperature.

14e. With the calorimeter on, the potential drops across the standard resistor and the voltage divider are measured with a D.C. voltmeter.

14f. When the desired amount of the feed material is added to the Dewar flask, the heater is turned off and injection of material is stopped. The temperature in the Dewar flask is reproduced to within ±0.0005°C of the set temperature.

14g. The readings of the stopwatch and the burette are recorded.

14h. Repeating steps 14b to 14g allows the determination of another data point on the heat of mixing curve.

The experiment is terminated when the calorimeter plug is at the top of the flask. Approximately 100 ml of the feed material is added to the flask over the course of one experimental run. Two experimental runs are necessary to completely determine a heat of mixing curve. Half of the curve is obtained from an experiment in which one component is initially placed in the flask and the other in the feed storage bulb and burette. In the second run, these components are interchanged.

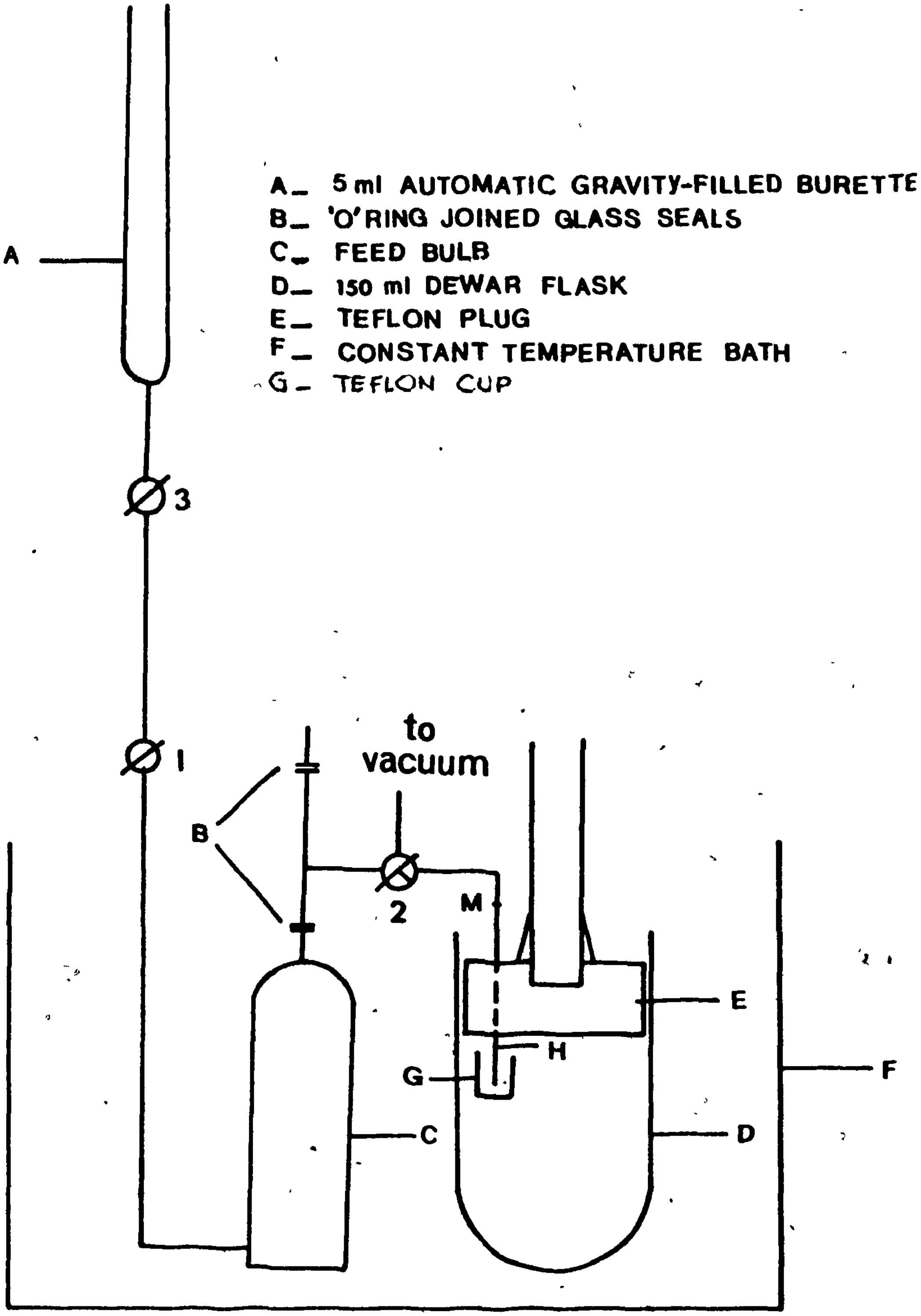
The heats of mixing are calculated from the following measurement:

- the mass of component 1 initially in the Dewar flask.
- the volume of component 2 injected into the Dewar flask.
- the potential drop across the standard resistor.
- the potential drop across the heater as measured across the voltage divider.
- the time interval during which the heater is operational.

Sample calculations of heats of mixing are shown in Appendix Al.

FIGURE 4.1

Schematic Diagram of the Calorimeter



A_ 5 ml AUTOMATIC GRAVITY-FILLED BURETTE
B_ 'O'RING JOINED GLASS SEALS
C_ FEED BULB
D_ 150 ml DEWAR FLASK
E_ TEFLON PLUG
F_ CONSTANT TEMPERATURE BATH
G_ TEFLON CUP

Schematic diagram of the calorimeter

FIGURE 4.2

Calorimeter Housing and Support

A. Stainless steel supporting tube for Teflon plug

B. Ball joint

C. Dewar vessel

D. Supporting framework for calorimeter

E. Threaded rod for the moving of Dewar vessel

F. Hand wheel

G. Rubber mold

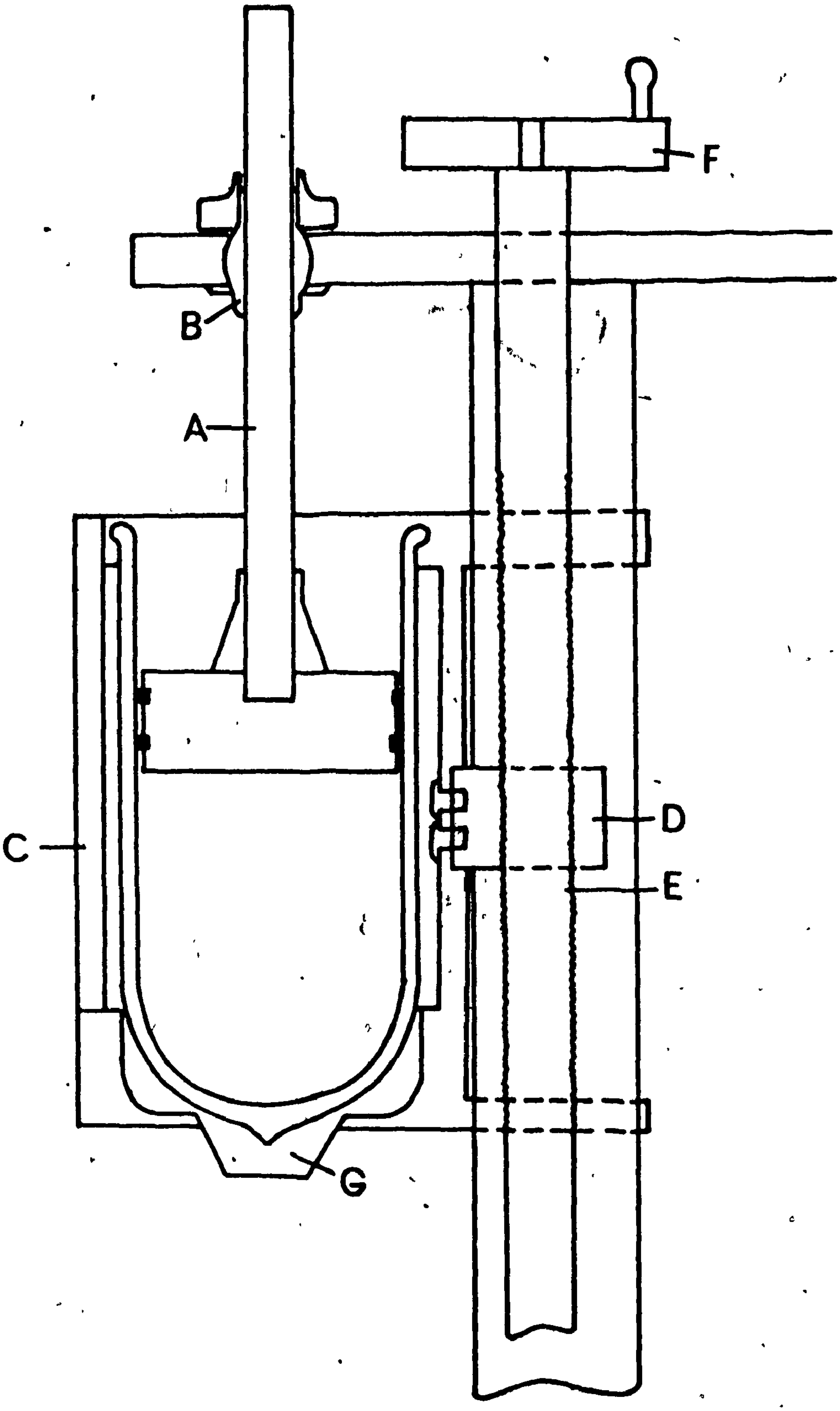

F
B
A
C
D
E
G

FIGURE 4.3

Calorimeter Plug - Side View

A. 150 ml. Precision bore Dewar flask

B. Teflon plug

C. Feed cup

D. Stainless steel hypodermic needle

E. Supporting tube for Teflon plug

F. Heater housing

G. Thermistor Housing

H. Stirrer paddle

I. Teflon-coated stirrer magnet

J. "O" rings

K. Vent screw

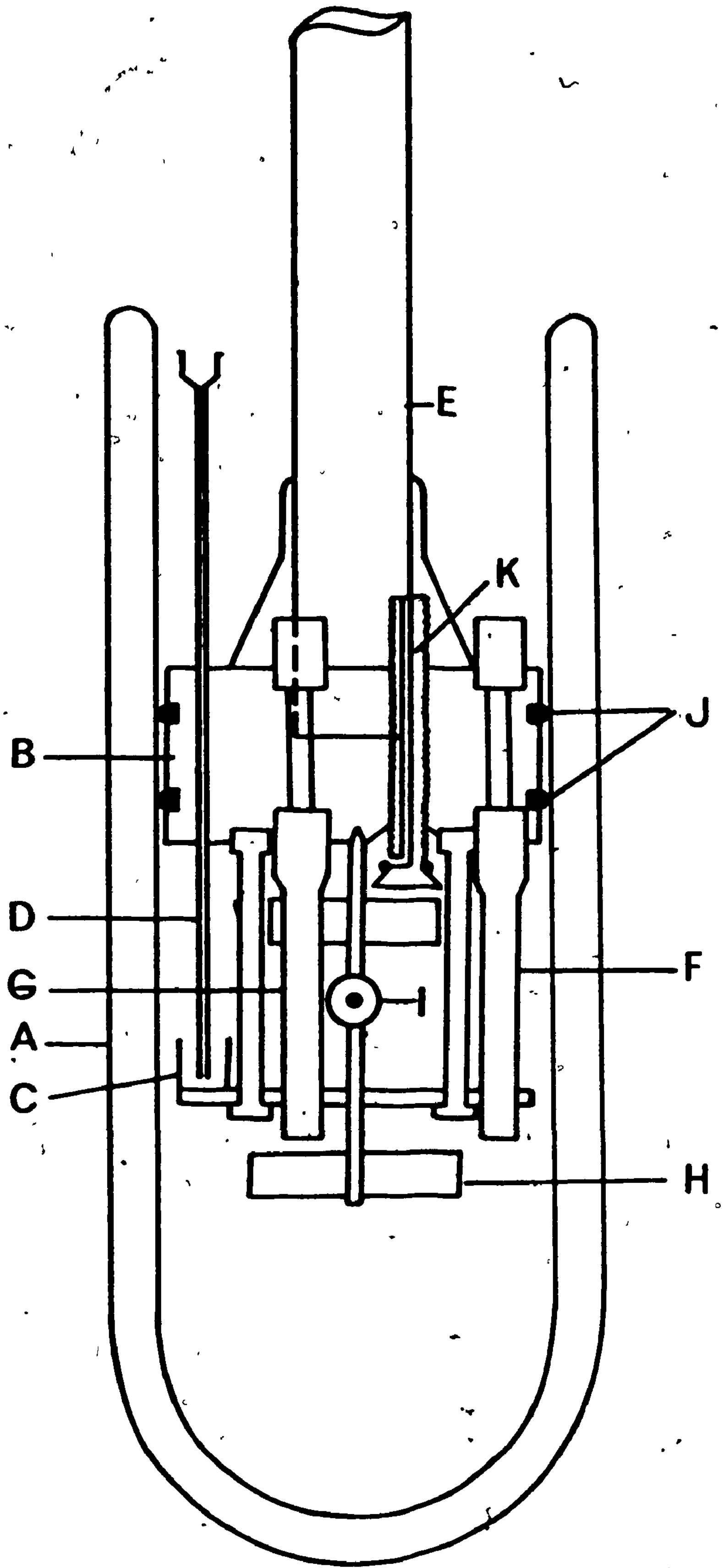
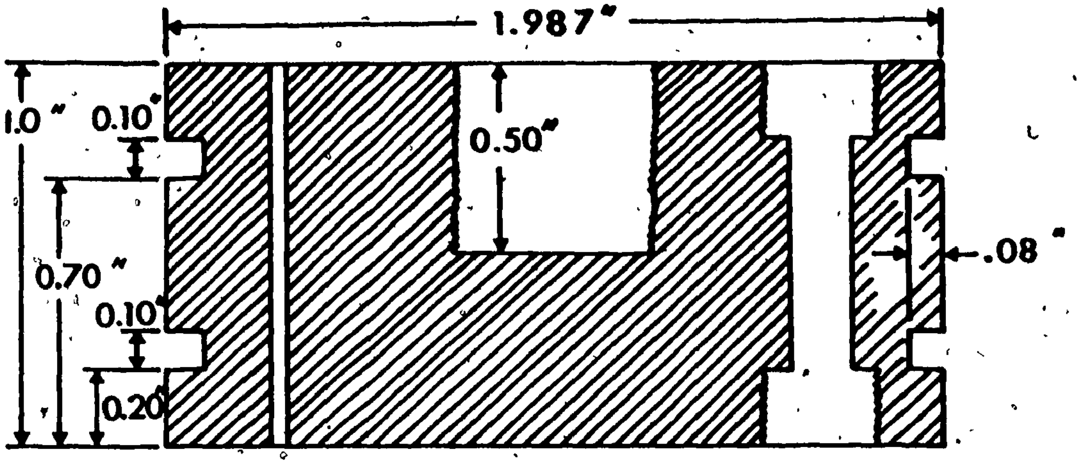

E
K
J
B
D
F
G
I
A
C
H

FIGURE 4.4

Calorimeter Plug - Detail


1.987"
1.0"
0.10"
0.50"
0.70"
0.10"
0.20"
.08"

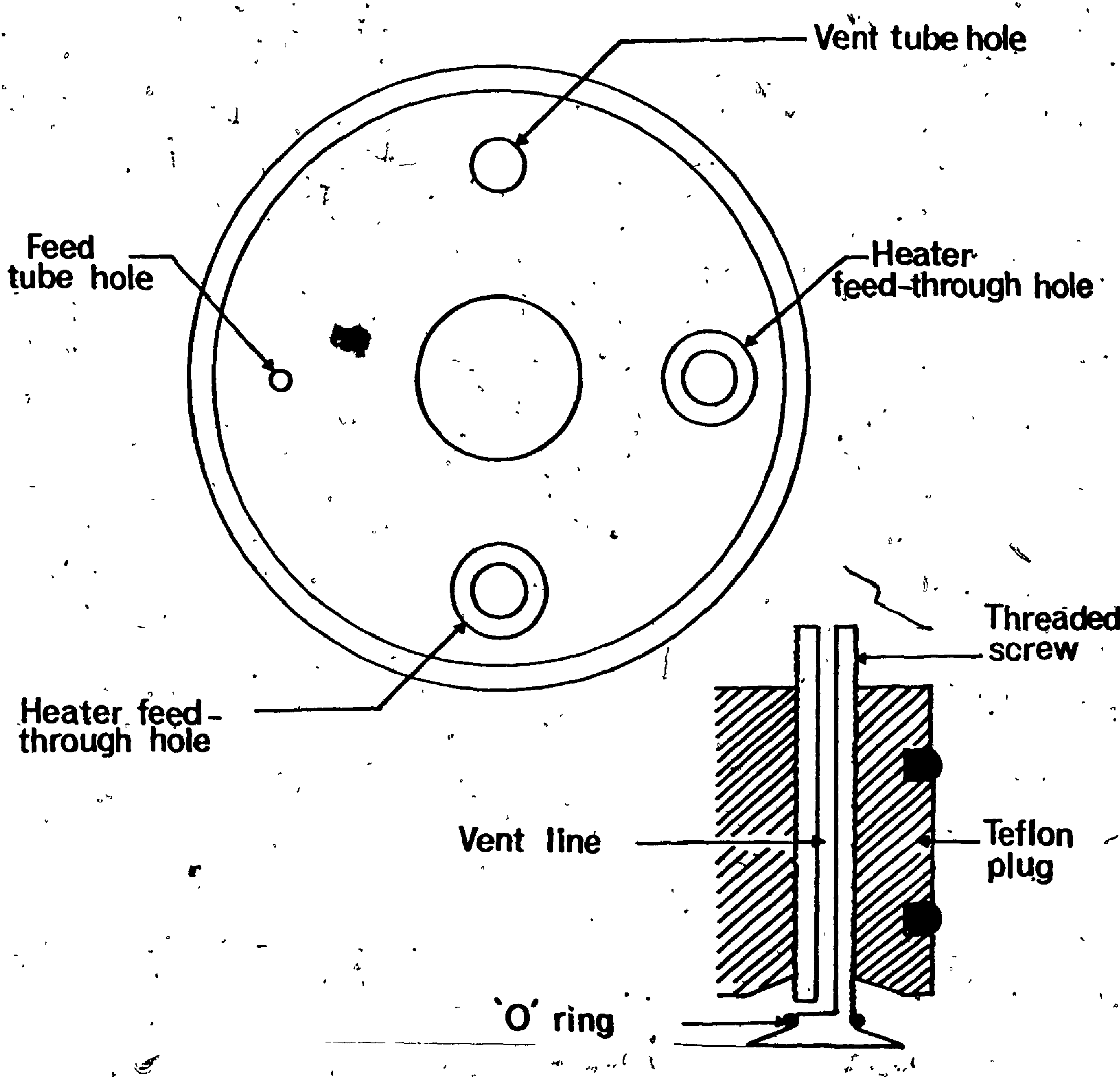
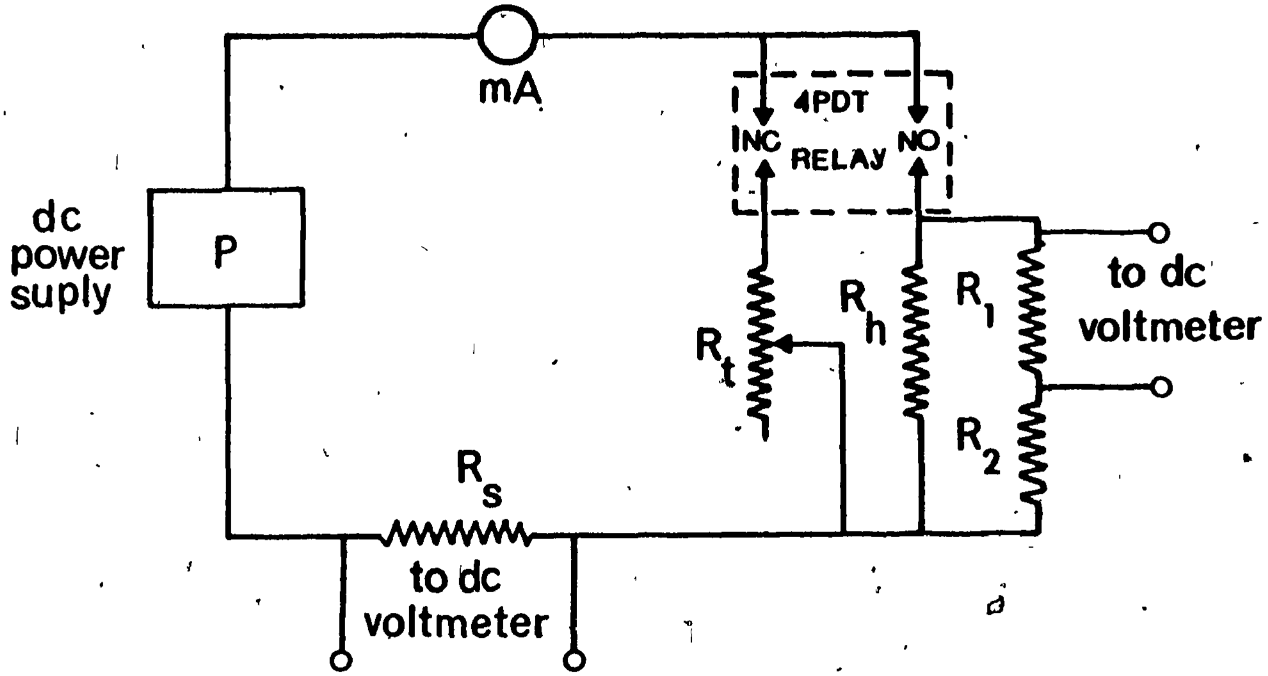
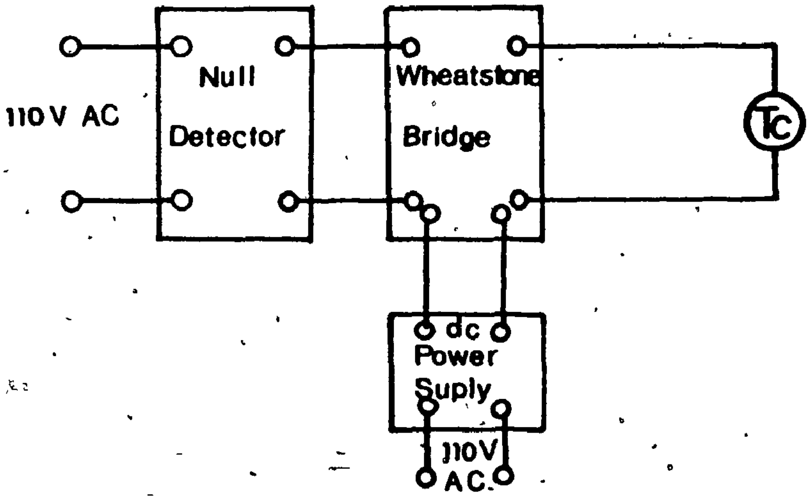

Vent tube hole
Feed tube hole
Heater feed-through hole
Heater feed-through hole
Threaded screw
Vent line
Teflon plug
'O' ring

FIGURE 4.5

Calorimeter Circuits



Calorimeter heater circuit



Thermistor circuit

FIGURE 4.6

General Lay-Out of the Calorimeter
Photograph

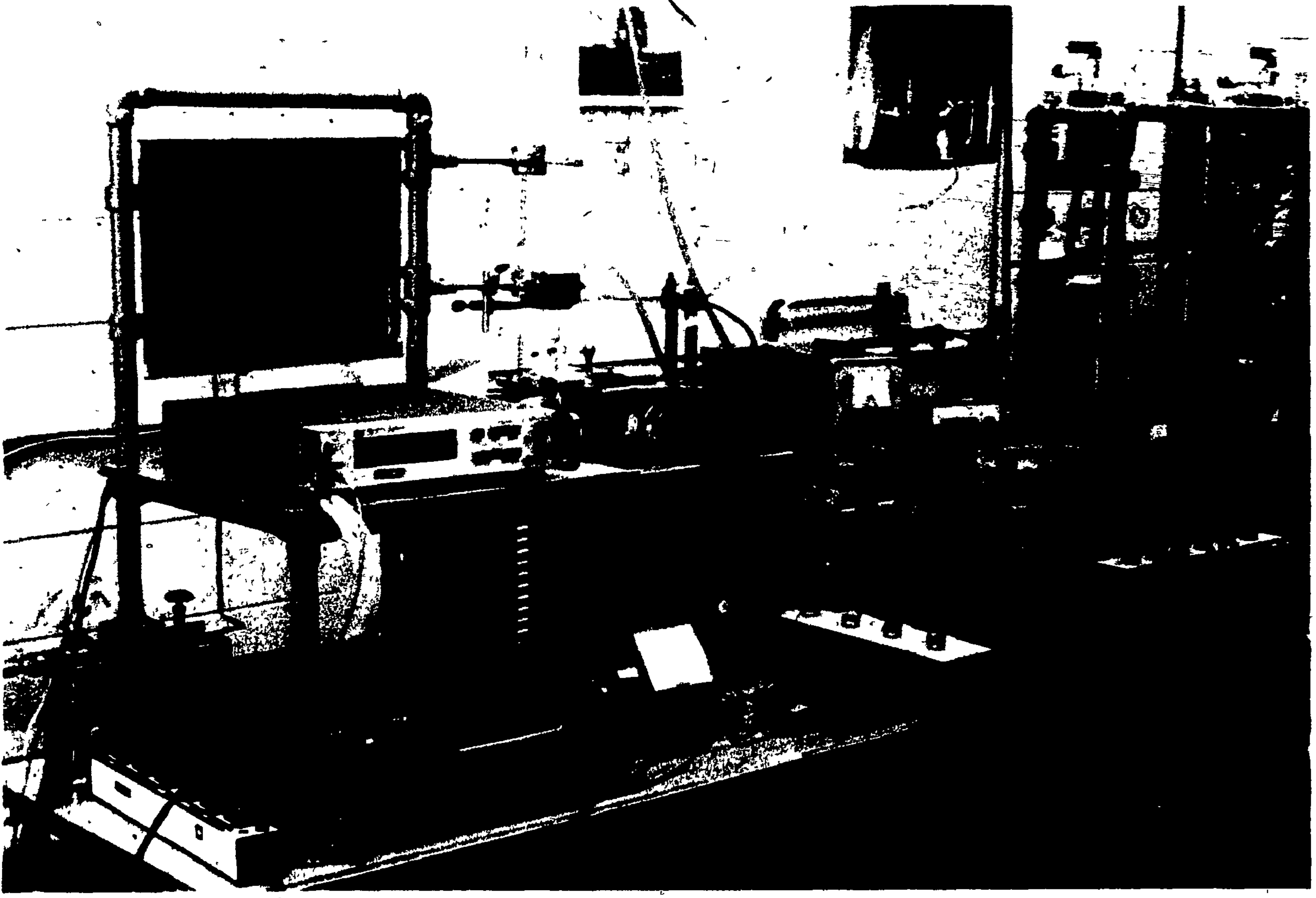
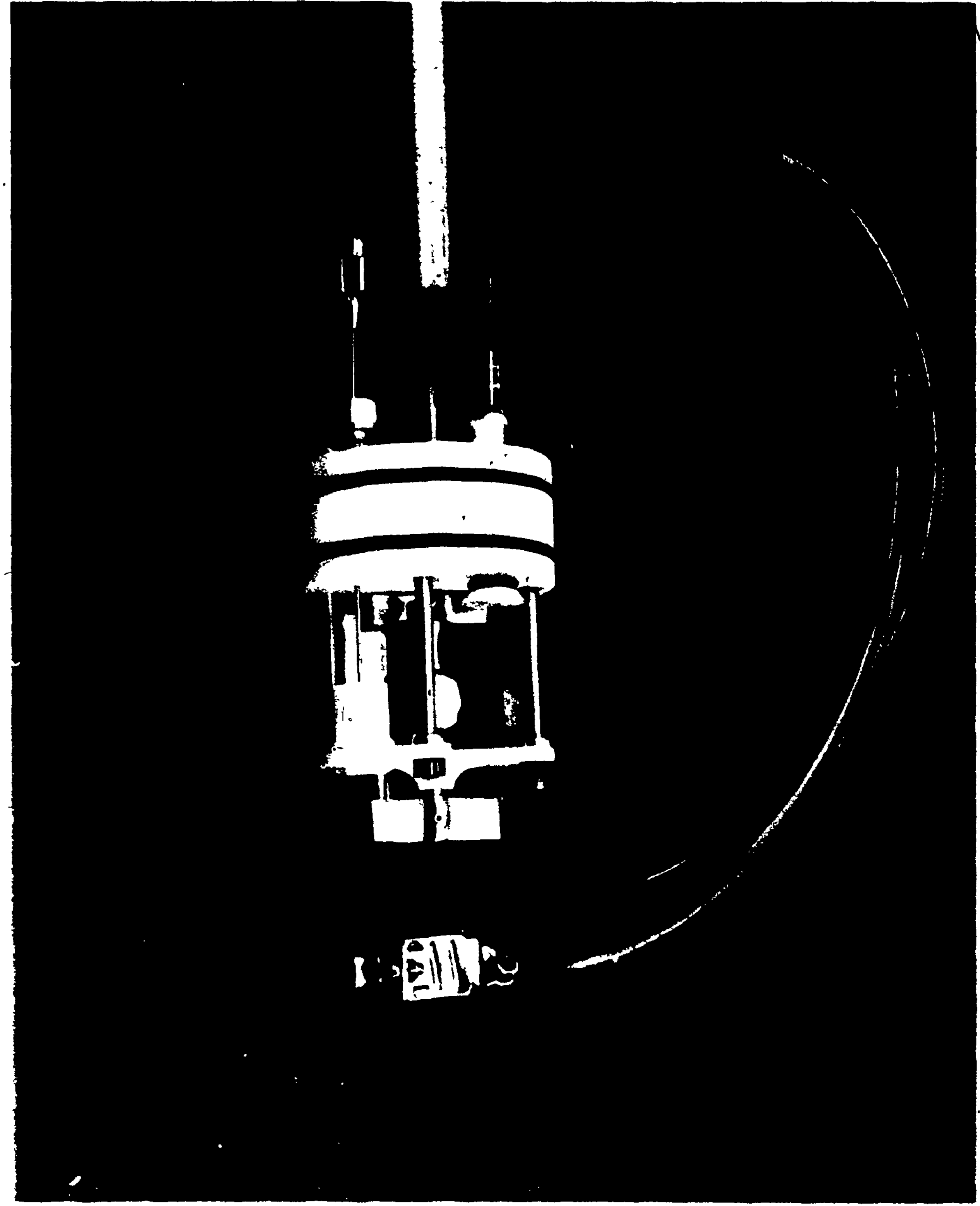


FIGURE 4.7

Calorimeter Plug - Photograph



5. MATERIALS

Specifications of all materials used in this study are listed in Table 5.1. The refractive indices of the materials were measured at 25°C with a Bausch and Lomb Precision Refractometer and are also tabulated in Table 5.1 along with values from literature.

All reagents had a purity in excess of 99 mole percent with the exception of n-hexanol which had a purity over 98 percent. As pointed out by Bennett and Benson (B5), the impurities which are the most difficult to remove from the reagents are not likely to effect the heats of mixing appreciably. Therefore, no attempt was made to achieve the utmost purity for the reagents.

TABLE 5.1

Materials-Supplier, Specifications and Refractive Indices

Material	Supplier	Specification	n_D(Meas. 25°C)	n_D^* (Lit.)
n-butanol	Aldrich Chemical Co.	Pure grade, 99 mole %	1.3970	1.3973
n-pentanol	Aldrich Chemical Co.	99 mole %	1.4079	1.4081
n-hexanol	Aldrich Chemical Co.	98 mole %	1.4160	1.4161
n-octanol	Aldrich Chemical Co.	99 mole %	1.4276	1.4275
iso-pentanol	Matheson, Colemann and Bell	Chromatoquality 99+ mole %	1.4046	1.4051
n-pentane	Phillips Petroleum Co.	Pure grade, 99^+ mole %	1.3547	1.35472
n-hexane	Phillips Petroleum Co.	Pure grade, 99^+ mole %	1.3725	1.37226
n-heptane	Phillips Petroleum Co.	Pure grade, 99^+ mole %	1.3850	1.38511
n-octane	Phillips Petroleum Co.	Pure grade, 99^+ mole %	1.3954	1.39505
n-nonane	Phillips Petroleum Co.	Pure grade, 99^+ mole %	1.4034	1.40311
n-decane	Phillips Petroleum Co.	Pure grade, 99^+ mole %	1.4096	1.40967
n-dodecane	Phillips Petroleum Co.	Pure grade, 99^+ mole %	1.4196	1.41949
benzene	Phillips Petroleum Co.	Pure grade, 99^+ mole %	1.4979	1.4976
cyclohexane	Phillips Petroleum Co.	Pure grade, 99^+ mole %	1.4235	1.4232

TABLE 5.1 (cont'd)

Material	Supplier	Specification	n_D(Meas.) 25°C	n_D^* (Lit.)
2,2-dimethylbutane	Phillips Petroleum Co.	Pure grade, 99^+ mole %	1.3662	1.36595
2,3-dimethylbutane	Phillips Petroleum Co.	Pure grade, 99^+ mole %	1.3723	1.37231
2-methylpentane	Phillips Petroleum Co.	Pure grade, 99^+ mole %	1.3687	1.36873
3-methylpentane	Phillips Petroleum Co.	Pure grade, 99^+ mole %	1.3739	1.37386

(*) A.P.I., Volume 1, Refractive Indices at 25°C

6. EXPERIMENTAL RESULTS

6.1 Experimental Results

Heats of mixing were measured for many aliphatic alcohol/alkane systems at 15°C, 25°C and 55°C and are reported in Table 6.1. The 36 sets of data on heats of mixing are tabulated both as $\Delta H/x_1x_2$ and ΔH versus concentration and are shown in Appendix A2. Some of the experimental results are graphically represented by the functions $\Delta H/x_2x_1$ and ΔH versus x_1 in Figures 6.1 through 6.5. As pointed out by Van Ness (V1), representation of heat of mixing measurements by the $\Delta H/x_1x_2$ function is very advantageous because it gives a very sensitive indication of the precision of the data.

The alcohol/hydrocarbon mixing process results in a large endothermic effect. This is largely the result of dissociation of the hydrogen-bonded alcohol structure in the hydrocarbon solvent. The dissociation process consumes a large amount of energy and the process is almost complete at relatively low alcohol concentration. Therefore, the heat of mixing curves are markedly asymmetric and ΔH usually passes through a maximum at an alcohol mole fraction of 0.2-0.3.

TABLE 6.1

Experimental Results

Systems	Temperature, °C
n-butanol/n-hexane	15
n-butanol/n-heptane	15
n-butanol/n-octane	15
n-butanol/n-decane	15
n-pentanol/n-heptane	15
n-pentanol/n-decane	15
n-hexanol/n-heptane	15
n-hexanol/n-octane	15
n-octanol/n-heptane	15
n-octanol/n-octane	15
n-octanol/n-decane	15
n-butanol/n-heptane	55
n-butanol/n-octane	55
n-butanol/n-nonane	55
n-butanol/n-dodecane	55
n-hexanol/n-octane	55
n-pentanol/n-octane	55
n-pentanol/n-nonane	55
n-pentanol/n-dodecane	55
n-octanol/n-heptane	55
n-octanol/n-octane	55
n-octanol/n-nonane	55
n-octanol/n-dodecane	55
n-pentanol/n-hexane	25
n-pentanol/2,2-dimethylbutane	25
n-pentanol/2,3-dimethylbutane	25

TABLE 6.1 (cont'd)

Systems	Temperature, °C
n-pentanol/2-methylpentane	25
n-pentanol/3-methylpentane	25
isopentanol/n-hexane	25
isopentanol/2,2-dimethylbutane	25
isopentanol/2,3-dimethylbutane	25
isopentanol/2-methylpentane	25
isopentanol/3-methylpentane	25
isopentanol/n-heptane	25
isopentanol/n-octane	25

FIGURE 6.1

Heats of Mixing at 55°C for the system n-Octanol/n-Heptane

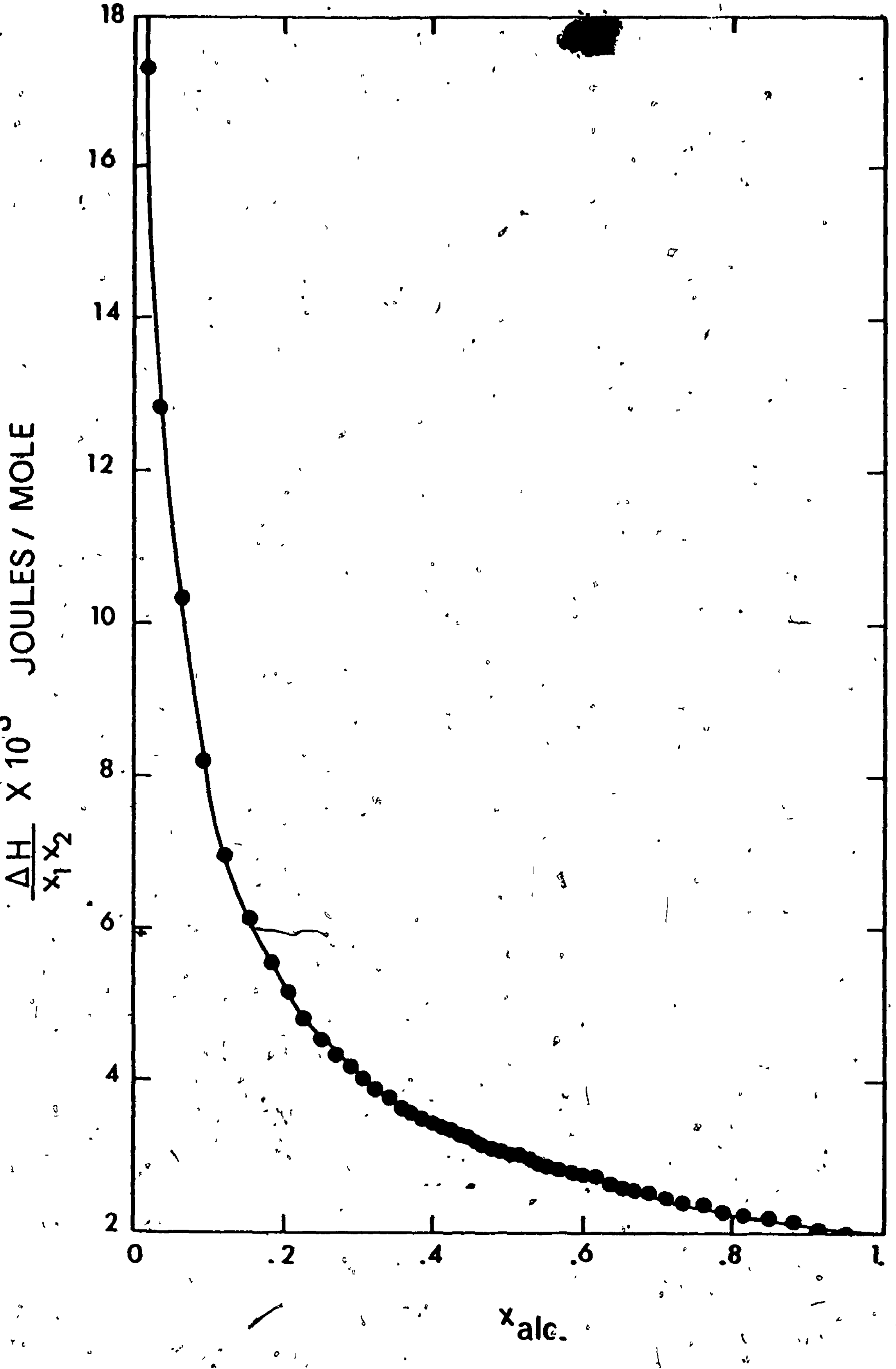

$\frac{\Delta H}{x_1 x_2}$ X 10^{-3} JOULES / MOLE
18
16
14
12
10
8
6
4
2
0
.2
.4
.6
.8
1
$x_{alc.}$

FIGURE 6.2

Heats of Mixing at 15°C for the System
n-Hexanol/n-Octane

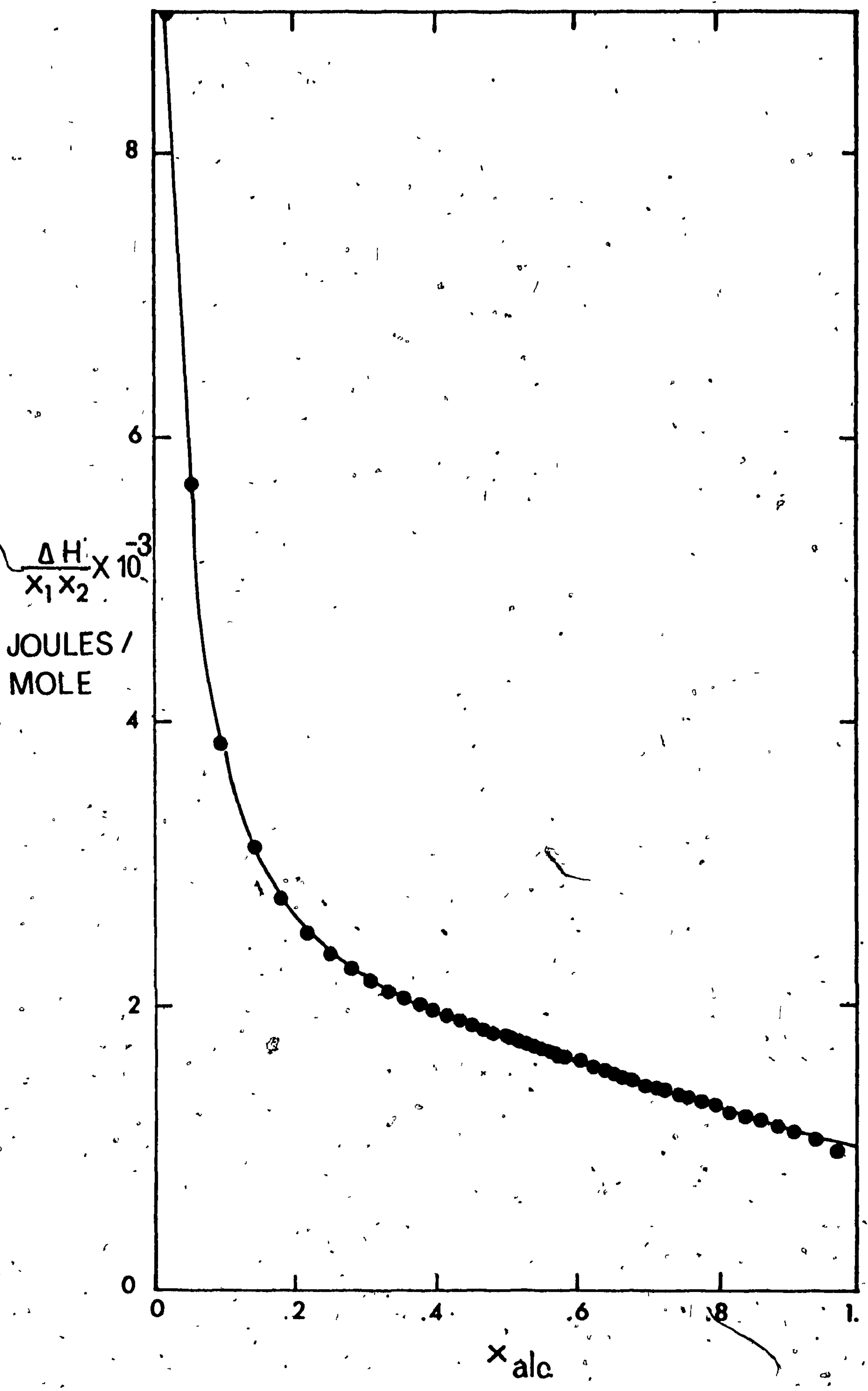
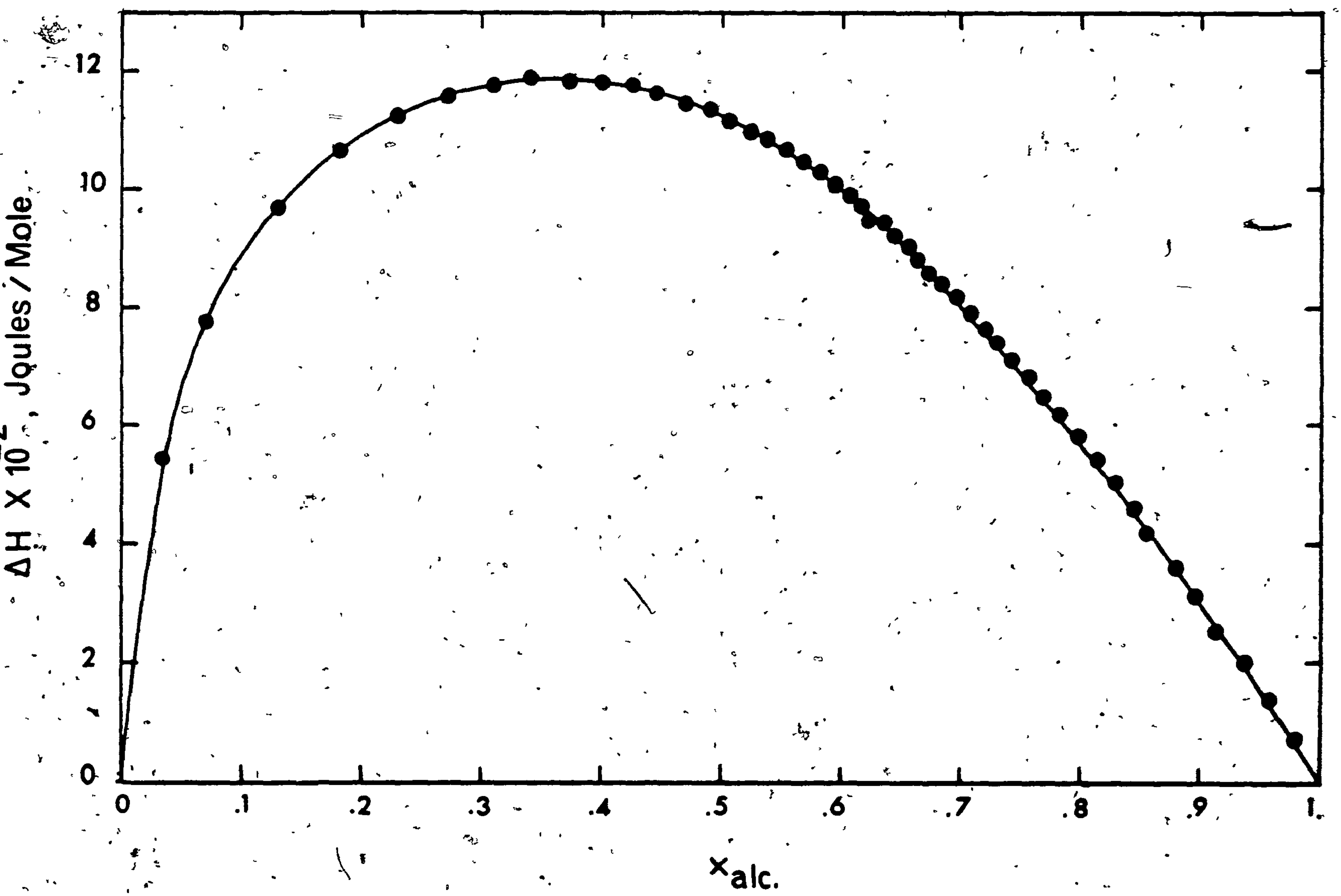

8
6
4
2
0
$\frac{\Delta H}{x_1 x_2} \times 10^{-3}$
JOULES / MOLE
0
.2
.4
.6
.8
1.
x_{alc}

FIGURE 6.3

Heats of Mixing at $55^{\circ}C$ for the System
n-Butanol/n-Octane



ΔH X 10^{-2}, Joules / Mole
0
2
4
6
8
10
12
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1.
$x_{alc.}$

FIGURE 6.4

Plot of ΔH vs $x_{alc.}$ at 15°C for the System n-Pentanol/n-Heptane

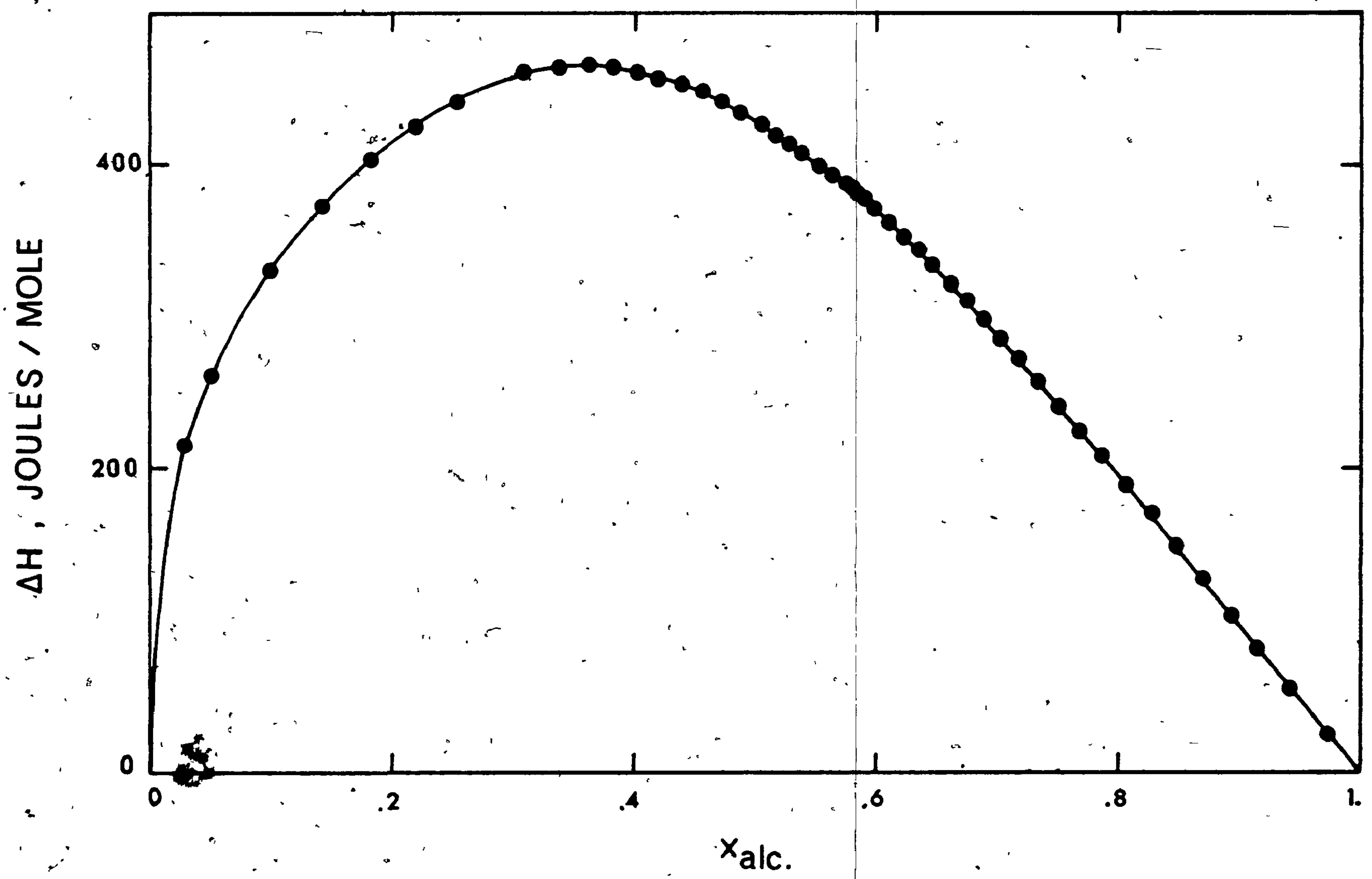
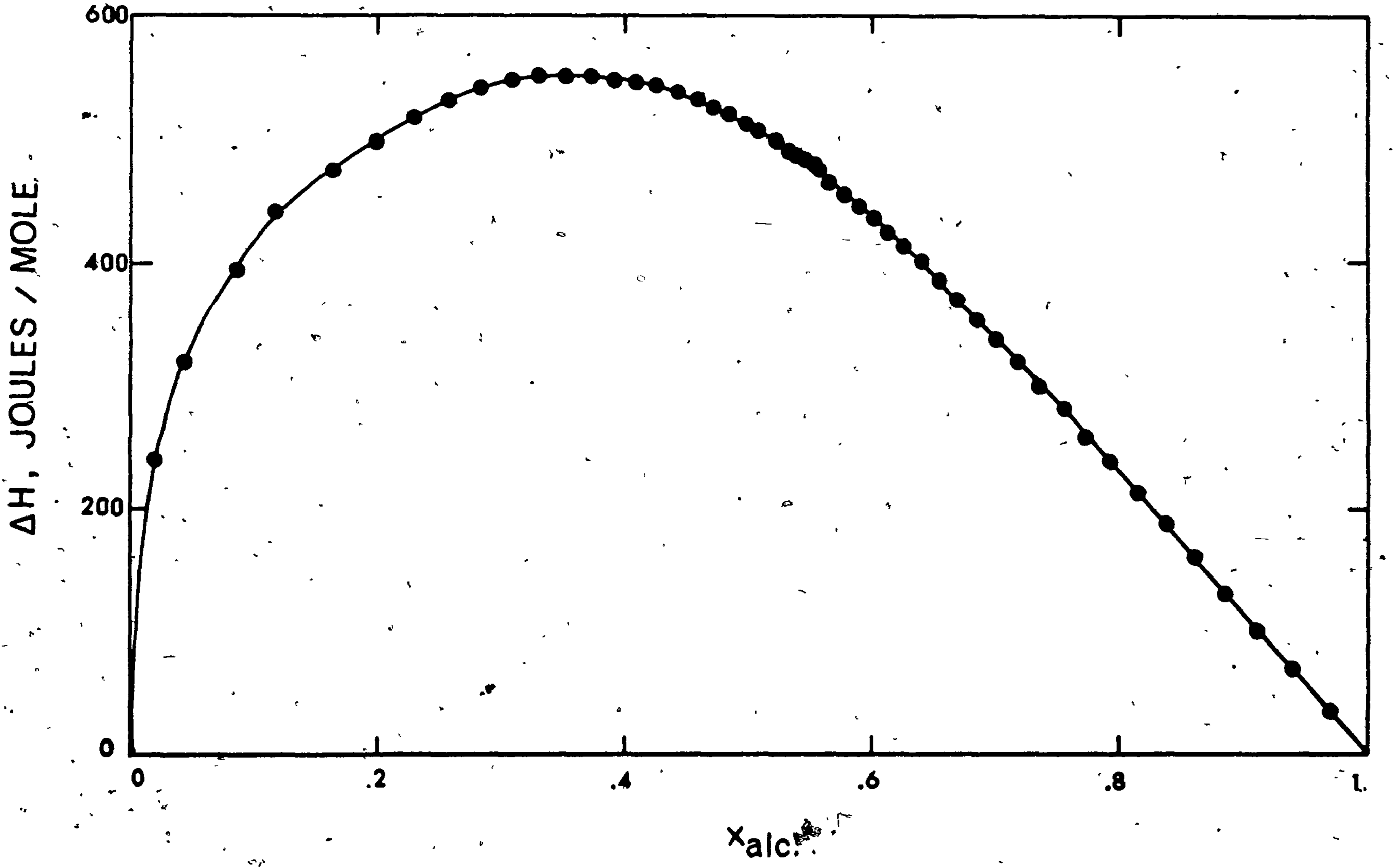

ΔH , JOULES / MOLE
400
200
0
0
.2
.4
.6
.8
1.
Xalc.

FIGURE 6.5

Plot of ΔH vs x_{alc} for the System Isopentanol/ 2-Methylpentane at 25°C


ΔH, JOULES / MOLE
600
400
200
0
0
.2
.4
.6
.8
1.
$X_{alc.}$

6.2 Discussions on Experimental Results

The isothermal, semi-continuous dilution calorimeter constructed in the course of this work permits rapid determination of heats of mixing for highly non-ideal alcohol/alkane systems. Direct association of the measured electrical energy input with the heats of mixing takes no account of any secondary effect which may enter during the mixing process. The secondary effects due to stirring have been discussed in details by Van Ness and Coworkers (S3). These effects will be briefly discussed with reference to Figure 6.6. This figure shows the Dewar flask, the feed bulb and the burette.

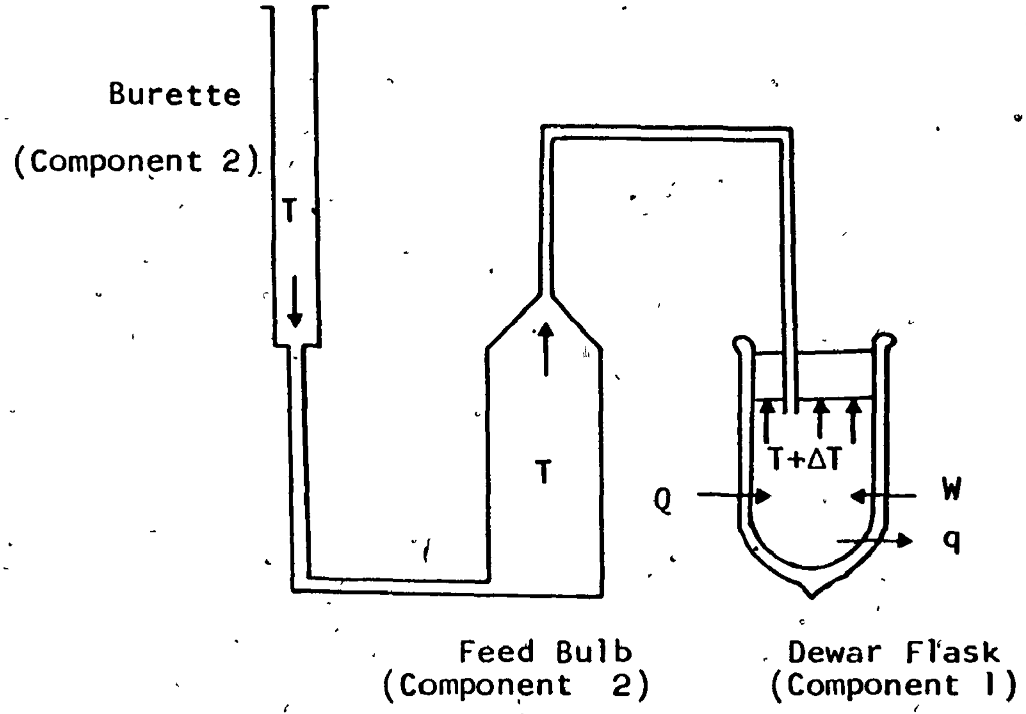


FIGURE 6.6
Energy Effects on the Calorimeter System during a Mixing Step

The thermodynamic system is taken as component 1 in the Dewar flask and component 2 in the feed bulb and the burette. Component 2 is to be injected into the Dewar flask. Pressure forces are exerted on the system by the liquid in the feed burette and the feed bulb and by the closure plug of the Dewar flask. These forces move during the mixing process and do work on the system. However, since they move slowly, their work effects essentially cancel.

The quantity W shown in Figure 6.6 represents the work of stirring. The steady stirring work raises the temperature in the Dewar flask by an amount of ΔT above that of the constant temperature bath during the equilibrium period. This ΔT is large enough as a heat transfer driving force so that the rate of heat transfer, q, from the Dewar flask to the bath just balances the energy input due to stirring. Since the energy input of stirring S is balanced by the energy loss by heat transfer q, no direct account need be taken of the stirring energy.

However, during mixing the energy supplied by the calorimeter heater Q must not only balance the heat of mixing but must also provide the sensible heat required to raise the temperature of the feed component from T to T + ΔT.

The energy input of stirring at constant stirrer speed is proportional to the density of the liquid in the

Dewar flask and thus ΔT is proportional to density. For highly non-ideal systems such as alcohol/hydrocarbon systems studied, the total heat Q for a run is about 300 to 400 cal., the densities are in the range 0.65 to 0.85 g/ml. In this case ΔT amounts to no more than 0.02°C and the heat capacities are about 0.5 cal./g, °C. Injection of about 70 grams of feed requires a sensible heat of about (0.5)(70)(0.02) = 0.7 cal. Thus the correction for the full run is less than 0.3% and need not, therefore, be made with great exactness. No other secondary effect of any significance is encountered in running the calorimeter.

Obtaining a good estimate of the accuracy for such a complex equipment as the calorimeter is extremely difficult. The best test of reliability of the calorimeter is, probably, to compare the results obtained with this instrument to the results obtained from other calorimeters. Heats of mixing of system benzene/cyclohexane have been studied by several investigators and therefore were chosen as data by which the performance of this calorimeter could be compared to others.

Figure 6.7 shows the heats of mixing for the system benzene/cyclohexane at 25°C as measured by Benson and Coworkers (M7) and Lundberg (L2) and this work. Data of Van Ness and Coworkers (S3) are represented by the fitted curve which has a root-mean-square deviation of 0.084% from experimental points.

FIGURE 6.7

Heats of Mixing at 25°C for the System Benzene/Cyclohexane

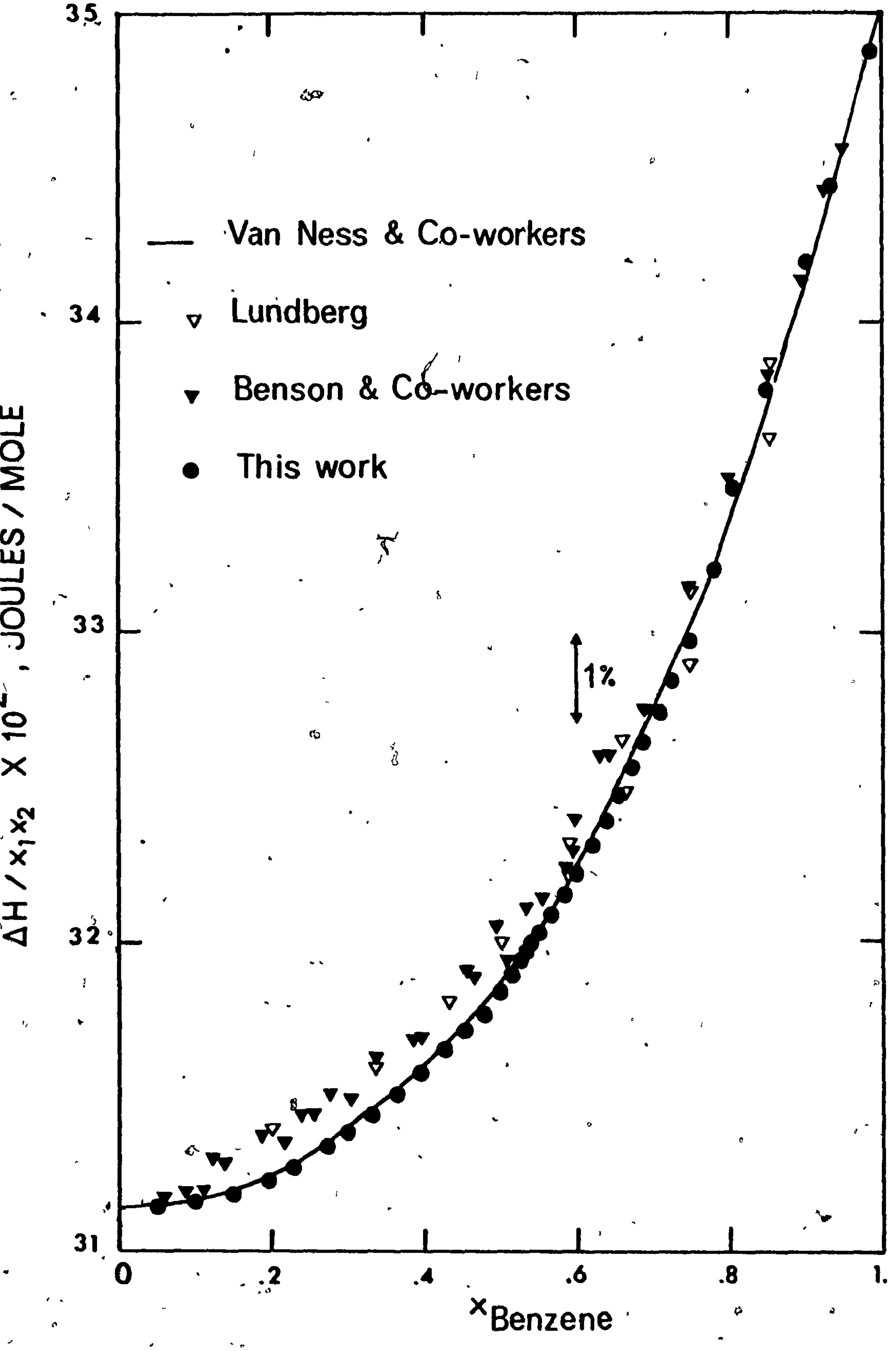

Van Ness & Co-workers
Lundberg
Benson & Co-workers
This work
1%
35
34
33
32
31
0
.2
.4
.6
.8
1.
$\Delta H / x_1 x_2 \times 10^{-2}$, JOULES / MOLE
x_{Benzene}

Figure 6.8 again compares the results taken in this work with those of Lundberg (L2) and Van Ness and Coworkers (S3) for the same system, but at 50°C.

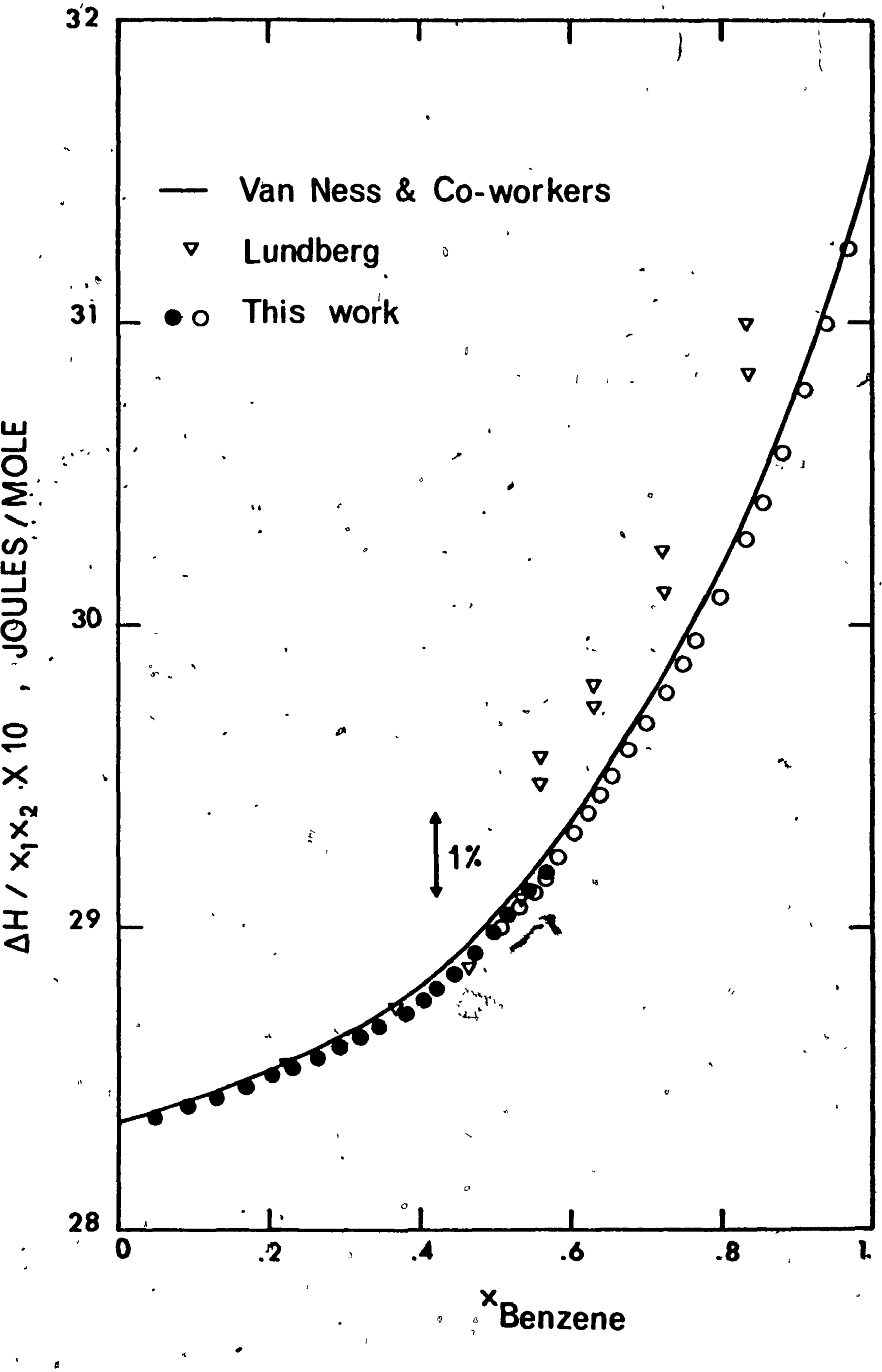
The reagent impurities might not account for the small discrepancies among the data. Bennett and Benson (B5) have made some experiments aimed at determining the effect of impurities on heats of mixing for the system benzene/carbon tetrachloride and found no significant difference between highly purified and the "reagent" grade materials as received from manufacturers.

There are, undoubtedly, systematic sources of errors in all calorimeters. Judging from the distributions of literature values shown in Figures 6.7 and 6.8, it seems reasonable to say that the values obtained with the present calorimeter fall within 1% of the true heats of mixing for the system benzene/cyclohexane at 25°C and 50°C.

The accuracy of the present calorimeter is, of course, very dependent on the types of systems investigated. For systems having small heats of mixing, a small fluctuation of the bath temperature may become very important while for systems having larger heats of mixing, the thermal gradients within the Dewar flask might present the biggest problem. In any event, for systems with heats of mixing not greatly different from those of benzene/carbon tetrachloride such as alcohol/hydrocarbon systems, it is quite reasonable to assume

FIGURE 6.8

Heats of Mixing at 50°C for the System
Benzene/Cyclohexane



Van Ness & Co-workers
Lundberg
This work
$\Delta H / x_1 x_2 \times 10^{-2}$, JOULES / MOLE
32
31
30
29
28
0
.2
.4
.6
.8
1.
1%
$x_{Benzene}$

that the heat of mixing data obtained with this calorimeter are within 1% of the true values.

The systems which have been studied in this work were chosen primarily for the purpose of evaluating the temperature dependency of the group Wilson parameters. However, some observations may be made which might be of some significance.

For all the aliphatic alcohol/alkane systems studied, the heats of mixing increase with increasing temperature. Heats of mixing also increase with increasing difference in the number of carbon atoms in the constituents. Generally speaking, if the number of carbon atoms in the n-alkane component is fixed, the heats of mixing decrease with an increase in the number of carbon atoms in the alcohol components.

Three types of behaviours are observed for the branched pentanol/hexane mixtures. When both the alcohol and alkane molecules have branching in the alkyl group, e.g. in the system isopentanol/2,2-dimethylbutane..., the branching does not have any effect on heats of mixing, that is, the system isopentanol/2,2-dimethylbutane has almost the same heats of mixing as the system n-pentanol/n-hexane. For systems containing a branched alcohol molecule and a n-alkane, the heats of mixing are a few percent higher than those of the equivalent n-alcohol/n-alkane system. The reverse is observed for branched alcohol/n-alkane systems, i.e., their heats of mixing are slightly lower than those of the equivalent n-alcohol/n-alkane mixtures.

Thus moderate branching in the cases studied has only a small effect on heats of mixing. One may expect these effects to be significant as found in alcohol/alkane systems containing secondary and tertiary alcohols (B6) where branching occurs in the vicinity of the polar group in the alcohol molecules.

7. APPLICATION OF THE ANALYTICAL GROUP SOLUTION MODEL TO ALCOHOL/ALKANE MIXTURES

The introduction of the analytical Wilson equation in the group solution model for heats of mixing provides a potentially powerful tool for correlating and predicting heat of mixing data.

Isothermal heats of mixing of n-alcohol/n-alkane systems found in the literature at 30°C and 45°C (S1-3) and those obtained from this work at 15°C and 55°C were used as reference data to study the temperature dependence of the model parameters.

7.1 Determination of Group Wilson Parameters From Excess Free Energies

Attempts to calculate heats of mixing using molecular parameters computed from vapor-liquid equilibrium data have not been very successful. The method consists of using measured vapor-liquid equilibrium data to evaluate the parameters in semi-empirical equations which in turn are used to calculate heats of mixing using the well-known Gibbs-Helmholtz relation:

$$\Delta H^M = -T^2 \left(\frac{\partial G^E/T}{\partial T}\right)_{P,x} \quad (7.1)$$

Thus, the error magnification inherent in differentiation of the basic experimental vapor-liquid equilibrium data can result in poor agreement between calculated and measured heats of mixing.

It has been found that group Wilson parameters computed from vapor-liquid equilibrium data (R3) can not be used to predict heats of mixing. One reason for the poor agreement is inherent in the results of the temperature dependency of the group Wilson parameter, $a_{CH_2/OH}$, computed from vapor-liquid equilibrium data for alcohol/alkane mixtures, i.e. mixtures formed from methylene and hydroxyl groups (methylene and methyl groups being assumed equivalent),

$$a_{OH/CH_2} = \exp(7.55 - 3800/(t + 273.16)) \quad (7.2)$$

$$a_{CH_2/OH} = 0.5 \quad (7.3)$$

t is in degree C.

Since $a_{CH_2/OH}$ is independent of temperature (equation (7.3)) the analytical expressions for group excess enthalpies, H_{CH_2} and H_{OH}, described by equations (3.20a) and (3.20b) are reduced to:

$$H_{CH_2}/RT^2 = X_{OH}^2 \frac{\partial}{\partial T}(a_{OH/CH_2})/(X_{OH}+X_{CH_2}\, a_{OH/CH_2})^2 \qquad (7.4)$$

$$H_{OH}/RT^2 = X_{CH_2}^2 \frac{\partial}{\partial T}(a_{OH/CH_2})a_{OH/CH_2}/(X_{OH}+X_{CH_2}a_{OH/CH_2})^2 \qquad (7.5)$$

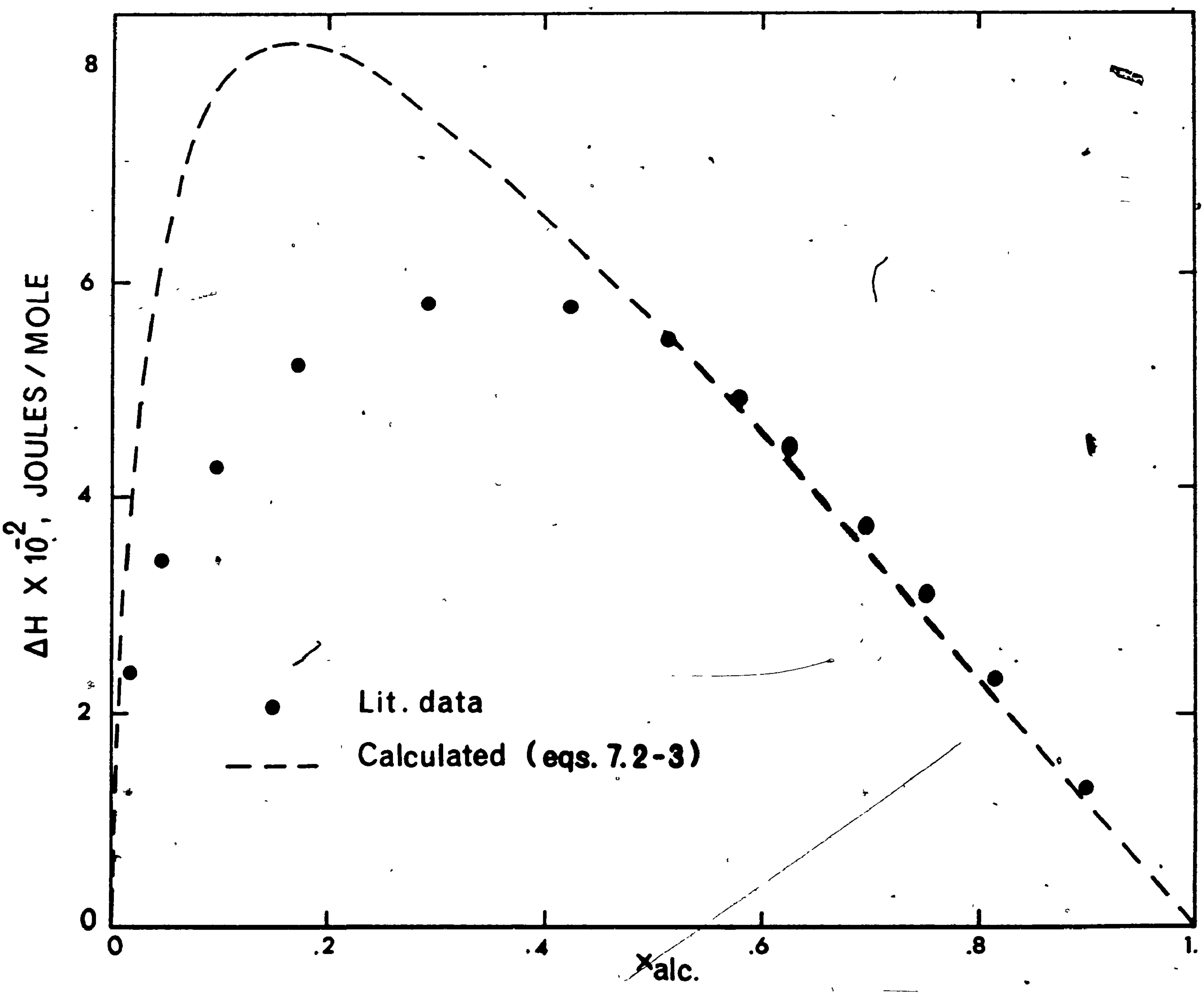
Heats of mixing for n-alcohol/n-alkane systems computed from equations (7.2-5) and (3.17-18) exhibit a very skew shape for the ΔH^M versus x plot. One example is shown in Figure 7.1 where heats of mixing are plotted against composition for the system n-pentanol/n-heptane (R6) at 25°C. The maximum of the computed curve occurs at a lower alcohol composition than the experimental.

Attempts were also made to estimate a_{OH/CH_2} and its temperature derivatives directly from experimental heats of mixing, using equations (7.4) and (7.5). Unfortunately, the results found indicated that the expressions (7.4) and (7.5) can not represent heats of mixing for n-alcohol/n-alkane mixtures because of the skew shape of ΔH^M versus concentration that these two expressions could give.

As will be apparent later, even though heats of mixing are very insensitive to variation in the value of $a_{CH_2/OH}$, as found by Ronc (R3) for excess free energies, it does not necessarily mean that this parameter is independent of temperature.

FIGURE 7.1

Heats of Mixing for the System n-Pentanol/ n-Hexane at 25°C


8
6
4
2
0
ΔH X 10^{-2}, JOULES / MOLE
0
.2
.4
.6
.8
1.
X$_{alc.}$
Lit. data
Calculated (eqs. 7.2-3)

Therefore, it was proposed to study the temperature dependence of the model parameters directly from heats of mixing for the aliphatic alcohol/alkane systems.

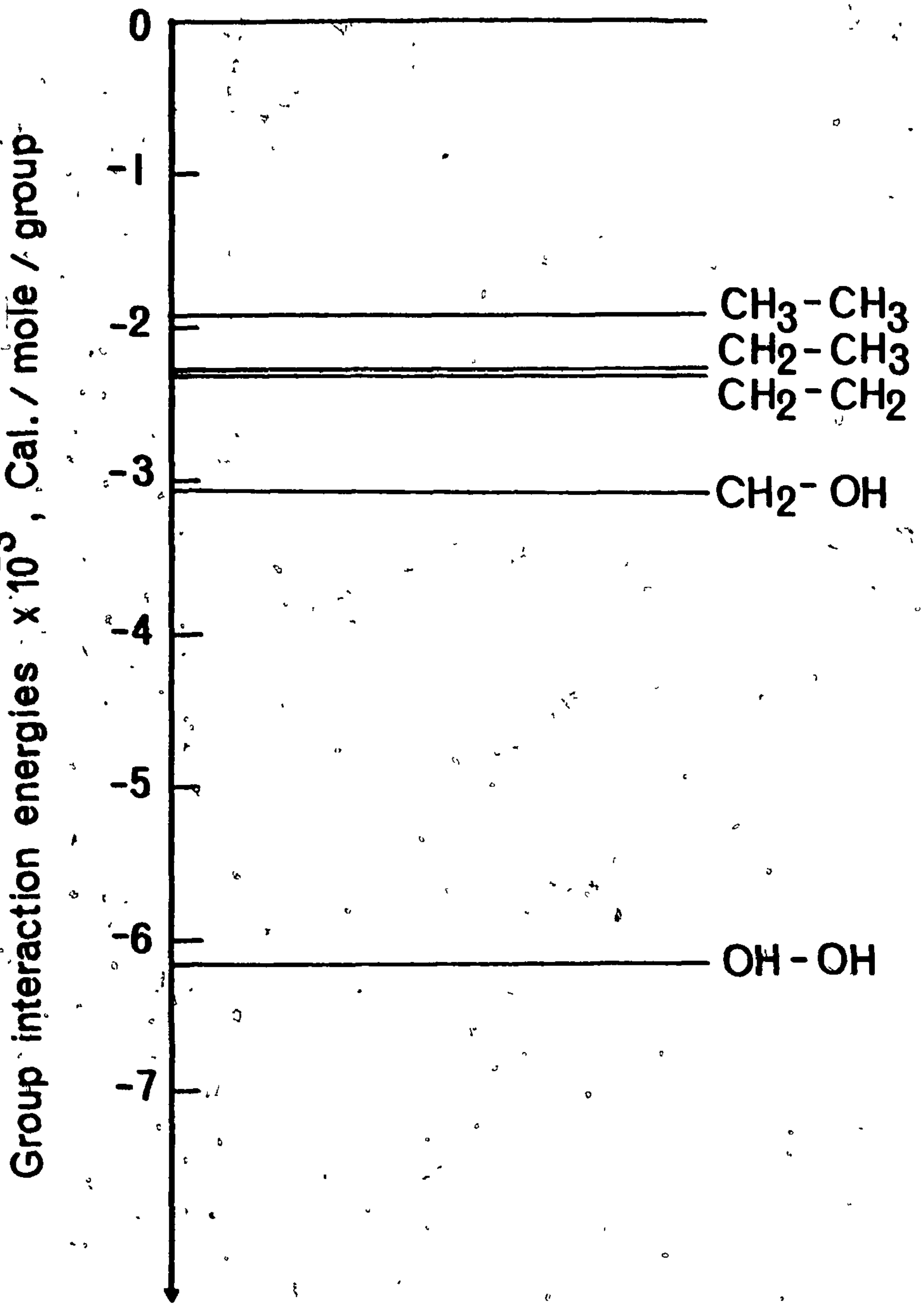
7.2 Determination of Group Wilson Parameters From Heats of Mixing

Wilson parameters for binary group mixtures of methylene and hydroxyl were determined for each of the eighteen n-alcohol/n-alkane systems at 15°C and 55°C using data collected during this work, and five such systems at 30°C and 45°C using the data of Van Ness and Coworkers (S1-3). As in previous work (N1-2), to preserve the simplicity of the model, no distinction is made between methylene and methyl groups, otherwise an alcohol/alkane mixture would be a ternary group system. This assumption seems reasonable in view of the group interaction energies computed at 30°C by Chao and Coworkers (C1) and shown in Figure 7.2 for various pairwise interaction groups; CH_2-CH_2, CH_2-CH_3, CH_3-CH_3, CH_2-OH, and OH-CH interaction energies.

The estimation of the group Wilson parameters in the non-linear model has been performed using the two best existing algorithms (J1): Marquardt algorithm (M5-6) and Spiral algorithm (J1). There were no significant differences between the least squares estimates of the parameters obtained from the two algorithms and it may be safely said that correct answers were obtained for the group Wilson parameters.

FIGURE 7.2

Group Interaction Energies in Alcohol/Alkane Mixtures at 30°C


Group interaction energies x 10^-3, Cal. / mole / group
0
-1
-2
-3
-4
-5
-6
-7
CH3-CH3
CH2-CH3
CH2-CH2
CH2-OH
OH-OH

The Marquardt program coded as GAUSS was obtained from the University of Wisconsin Computing Centre and the Spiral program from Shell's Thornton Research Centre. The Spiral program, originally written in FORTRAN V for the UNIVAC 1108, was converted to FORTRAN IV and only minor modifications were needed to adapt it to the IBM S360 of the McGill University Computing Centre. A brief description of the two programs is given in Appendix A3.

The group Wilson parameters were evaluated over the temperature range 15°C to 55°C for n-alcohol/n-alkane mixtures, and the values of the parameters were found to be:

$$a_{OH/CH_2} = 34.95 \exp(-2908/T) \qquad (7.6)$$

$$a_{CH_2/OH} = 26.69 \exp(-1336/T) + 7.705 \qquad (7.7)$$

It should be mentioned that the computed heats of mixing using the values of the group parameters given by equations (7.6) and (7.7), were found to be insensitive to the variation in $a_{CH_2/OH}$. This observation is very well indicated by the slight change of its values over the range of temperature studied (Table 7.1), i.e. from 7.96 to 8.16. Any value of that order used for $a_{CH_2/OH}$ would not effect the prediction accuracy. However, it should be emphasized that $a_{CH_2/OH}$ should not be fixed constant with respect to temperature, since this would result in equations (7.4) and (7.5)

TABLE 7.1

Group Wilson Parameters for Heats of Mixing of Alcohol/Alkane Systems

T°C	a_{OH/CH_2}	$\frac{\partial}{\partial T} a_{OH/CH_2}$	$a_{CH_2/OH}$	$\frac{\partial}{\partial T} a_{CH_2/OH}$
15	.00144	$.5046 \times 10^{-4}$	7.96305	.00416
30	.002373	$.7516 \times 10^{-4}$	8.0297	.00477286
45	.003732	1.0730×10^{-4}	8.1047	.005284
55	.004932	1.333×10^{-4}	8.1593	.005645

as described in section 7.1. Thus, even though heats of mixing are insensitive to the variation in the value of $a_{CH_2/OH}$, as found by Ronc (R3) for excess free energies, it does not necessarily imply that $a_{CH_2/OH}$ is temperature independent.

Use of the parameters given by equations (7.6) and (7.7) regenerated experimental heats of mixing for reference systems with an average root-mean-square deviation of less than 5%; details are given in Table 7.2. The calculated values for ΔH may be regarded as essentially predictions since the elimination of any one of the reference systems would not effect the best values of the parameters.

Figures 7.3 through 7.7 compare the prediction with experimental values. Prediction is as good in the case of ternary mixtures, as shown in Figure 7.7 for the system n-heptane/n-propanol/n-pentanol at 25°C (R6).

Predictions are poorer for lower alcohol/alkane mixtures such as ethanol systems for which the average root-mean-square deviation is about 15% (Table 7.3). The increased discrepancy for mixtures of lower alcohols in n-alkanes is related to their apparent anomalous behaviour shown in Table 7.4, where the heats of mixing of equimolar mixtures of various alcohols in n-hexane (B6) show a common trend for all alcohols except for ethanol and methanol. Brown, Fock and Smith (B6) attempted to explain this anomalous behaviour as

TABLE 7.2

Prediction Results on n-Alcohol/n-Alkane Systems

System	RMD(%) 15°C	RMD(%) 55°C
n-butanol/n-hexane	7.2	--
n-butanol/n-heptane	9.5	3.1
n-butanol/n-octane	3.5	2.5
n-butanol/n-nonane	--	3.3
n-butanol/n-decane	8.3	--
n-butanol/n-dodecane	--	5.1
n-pentanol/n-octane	3.1	--
n-pentanol/n-nonane	--	4.4
n-pentanol/n-decane	3.3	--
n-pentanol/n-dodecane	--	4.9
n-hexanol/n-heptane	9.0	--
n-hexanol/n-octane	6.6	2.7
n-octanol/n-hexane	6.5	--
n-octanol/n-heptane	7.6	2.8
n-octanol/n-octane	5.0	3.6
n-octanol/n-nonane	--	5.5
n-octanol/n-decane	5.9	--
n-octanol/n-dodecane	--	6.1
	30°C	45°C
n-propanol/n-heptane	3.9	2.6
n-butanol/n-heptane	2.7	4.0
n-pentanol/n-hexane	4.3	4.0
n-octanol/n-heptane	4.4	3.1
n-octanol/n-nonane	3.5	4.3

FIGURE 7.3

Prediction of Heats of Mixing for the System n-Pentanol/n-Decane at 15°C

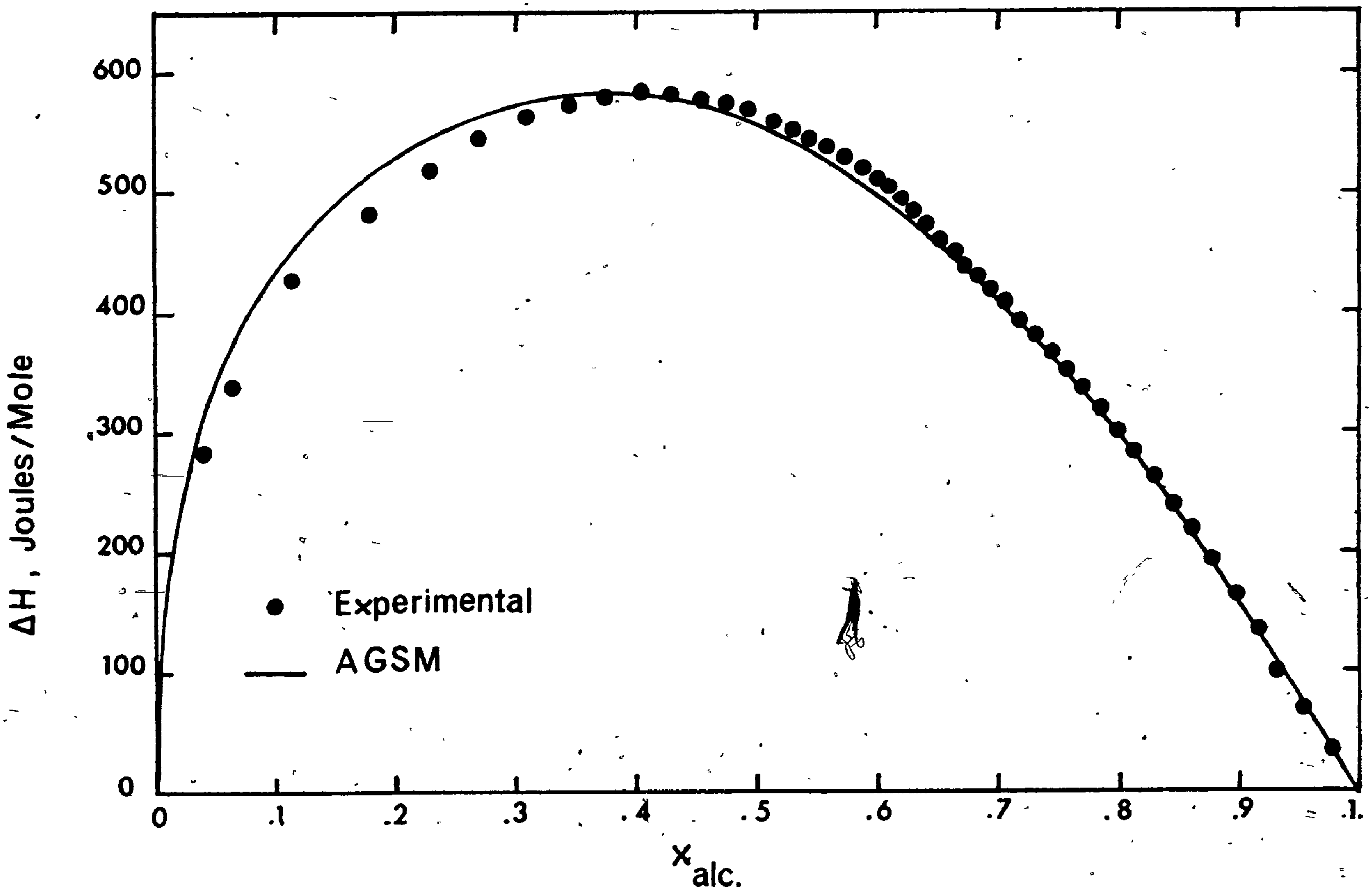

600
500
400
300
200
100
0
ΔH , Joules/Mole
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
.1.
$x_{alc.}$
● Experimental
— AGSM

FIGURE 7.4

Prediction of Heats of Mixing for the System n-Pentanol/n-Hexane at 30°C

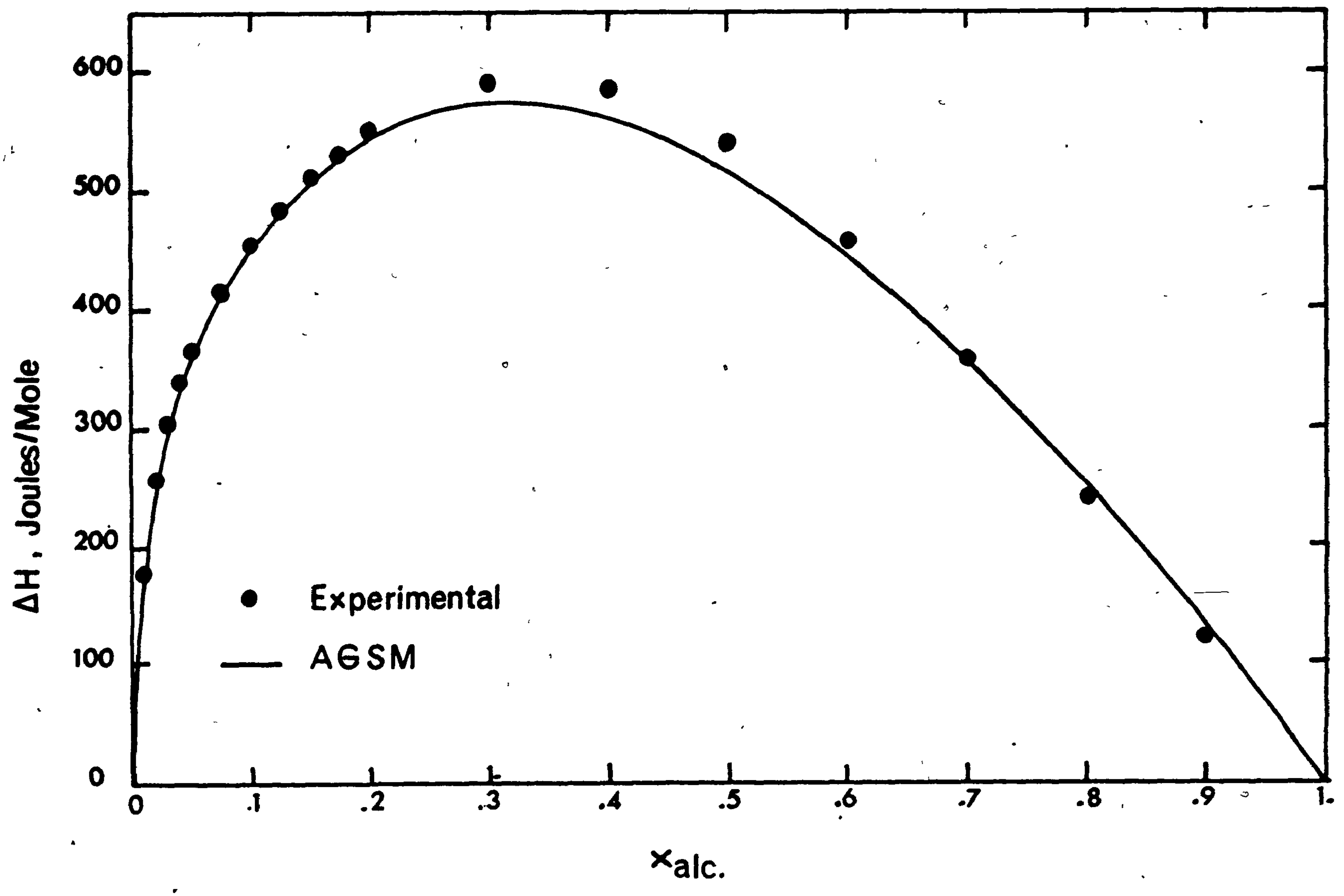

ΔH , Joules/Mole
600
500
400
300
200
100
0
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1.
Xalc.
● Experimental
— AGSM

FIGURE 7.5

Prediction of Heats of Mixing for the System n-Octanol/n-Nonane at 45°C

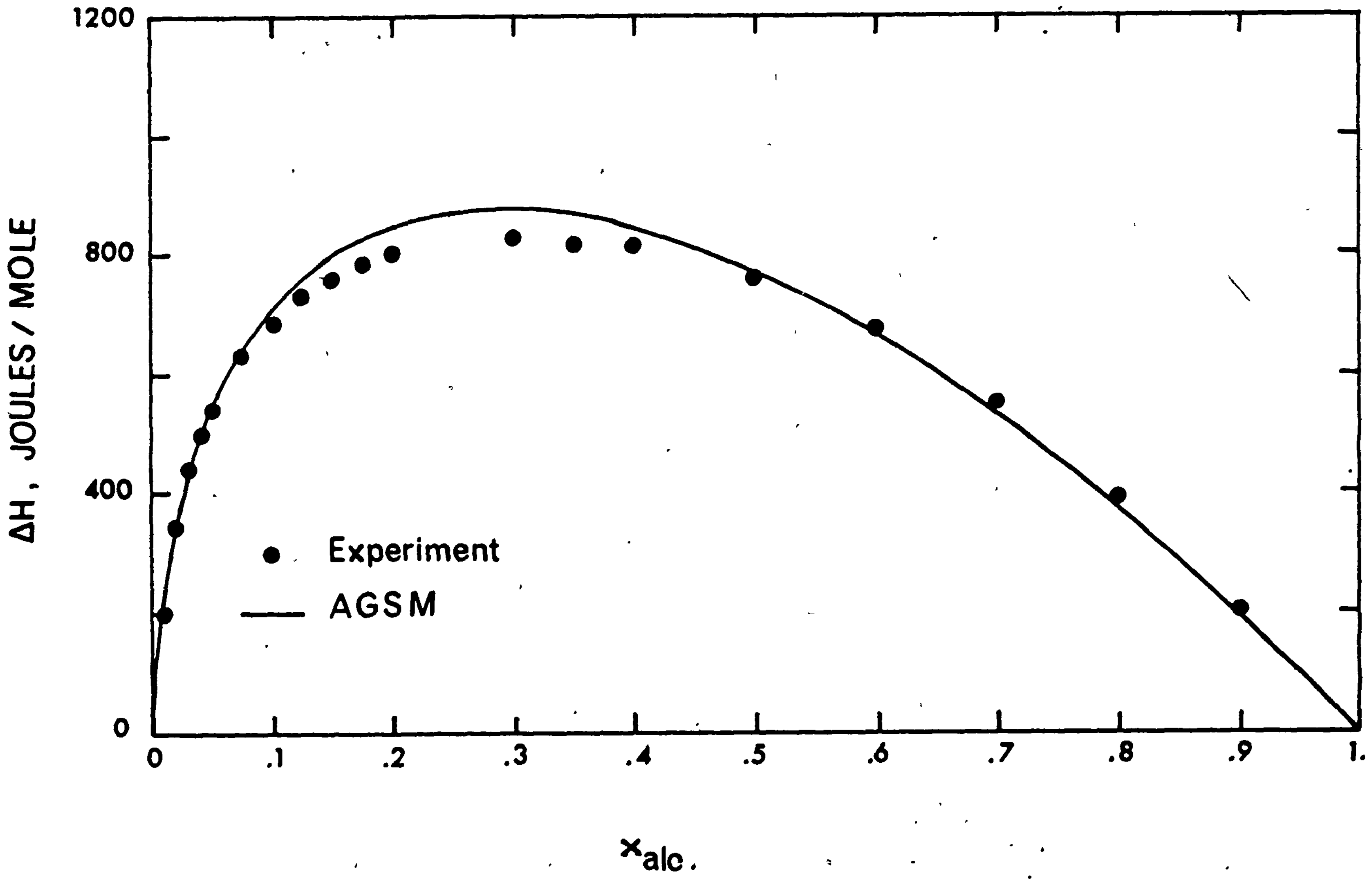

1200
800
400
0
ΔH, JOULES / MOLE
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1.
$x_{alc.}$
● Experiment
— AGSM

FIGURE 7.6

Prediction of Heats of Mixing for the System n-Pentanol/n-Octane at 55°C

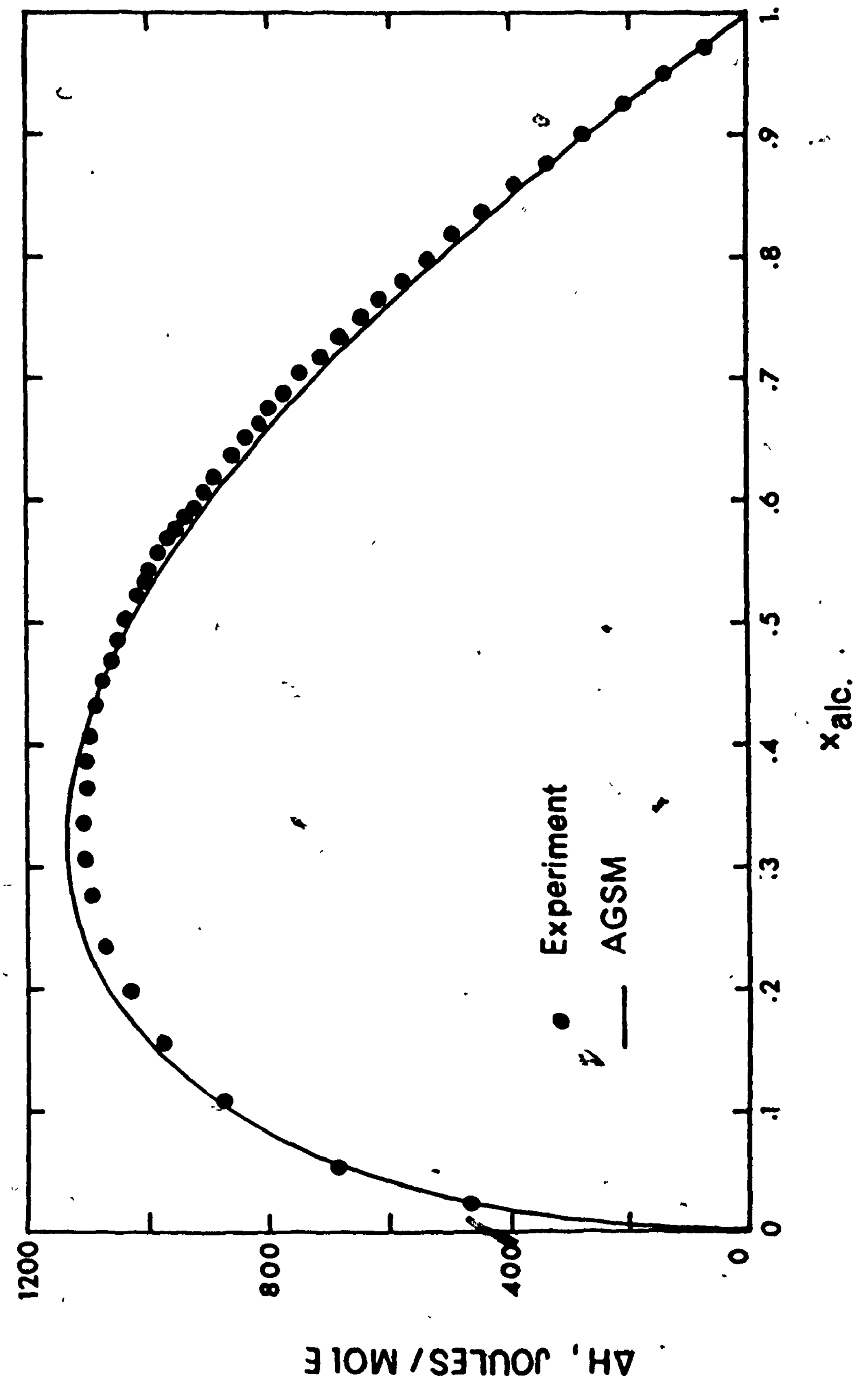

ΔH, JOULES/ MOLE
1200
800
400
0
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1.
$x_{alc.}$
● Experiment
— AGSM

FIGURE 7.7

Prediction of Heats of Mixing for the System n-Pentanol/n-Propanol/n-Heptane at 25°C

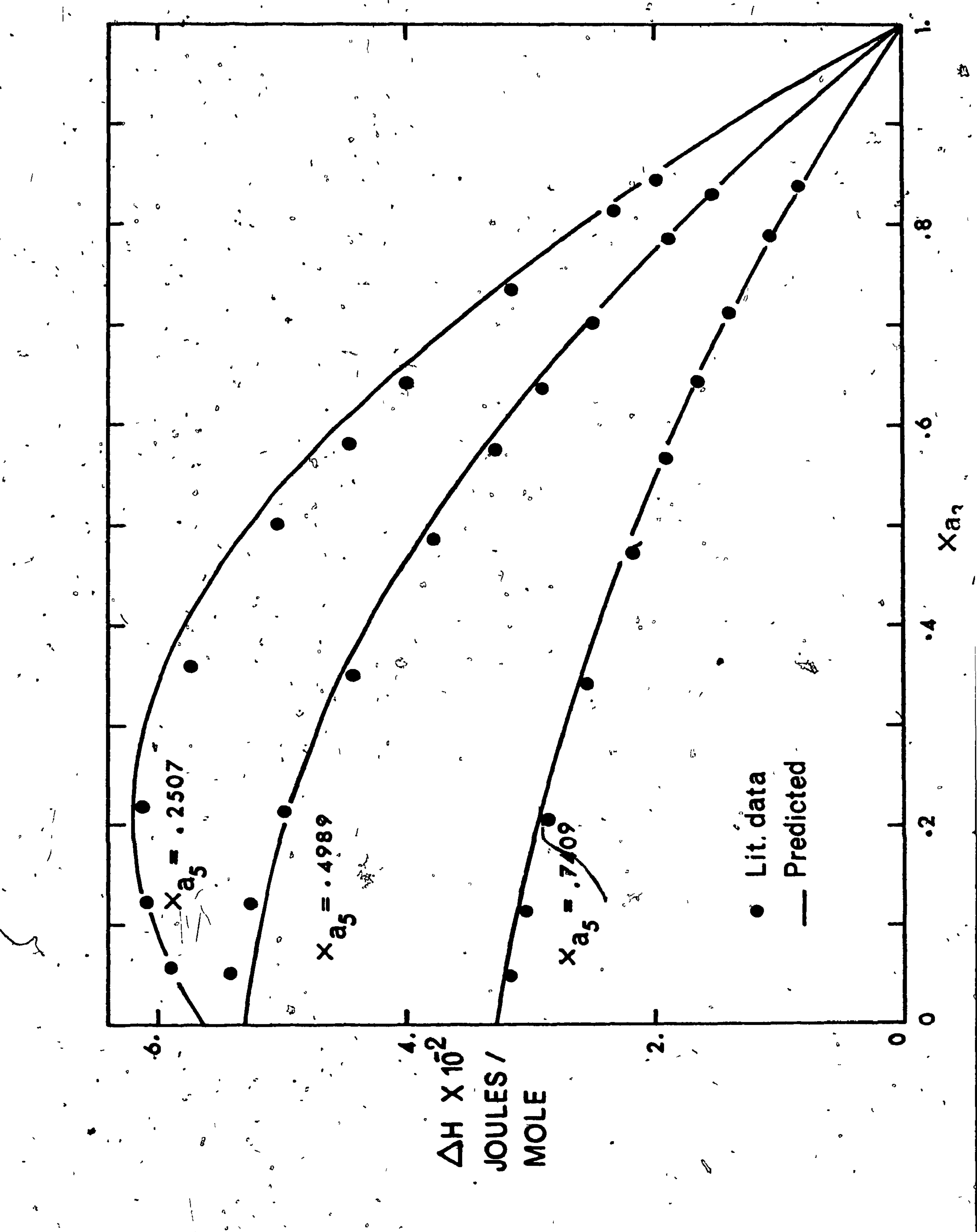

ΔH X 10⁻²
JOULES / MOLE
6.
4.
2.
0
0
.2
.4
.6
.8
1.
Xa₂
Xa₅ = .2507
Xa₅ = .4989
Xa₅ = .7409
● Lit. data
— Predicted

TABLE 7.3

Prediction Results on Ethanol/n-Alkane Systems

System	T(°C)	RMS Deviation (%)
ethanol/n-heptane	30	13.1
ethanol/n-hexane	30	11.3
ethanol/n-nonane	30	18.5
ethanol/n-hexane	45	10.9
ethanol/n-heptane	45	11.3
ethanol/n-nonane	45	22.3

TABLE 7.4

Heats of Mixing for Equimolar Mixtures of n-Alcohol/n-Hexane at 25°C (B6)

n-Alcohol	H^E J/mole^{-1}
methanol	500
ethanol	555
propanol	565
pentanol	570
hexanol	465
octanol	415

follows: in addition to the hydrogen bond contribution to heats of mixing, another contribution due to the mixing of the alcohol homomorph with the solvent was also important for the systems containing lower alcohols such as ethanol and methanol. This contribution accounts for the decrease in heats of mixing (Table 7.4) in systems containing lower alcohols.

7.3 Effect of Molecular Shape on Heats of Mixing

One of the limitations inherent in the group solution model is that the model does not take into account molecular shape. The model thus predicts identical heats of mixing for isomers. This effect of molecular shape on heats of mixing may be judged by inspecting the experimental heats of mixing of binary systems of n-pentanol or isopentanol with hexane isomers (2-methylpentane, 3-methylpentane, 2,2-dimethylbutane, 2,3-dimethylbutane). Table 7.5 shows the heats of mixing of these systems at 25°C at near equimolar composition. The small difference in heats of mixing of these systems suggests that there is only a small contact energy difference between methyl and methylene groups.

Most recently, Patterson (P5) has also made some study on the effect of the molecular shape on heats of mixing of alkanes of different molecular size. He measured heats of mixing for equimolar mixtures of alkane isomers of formula

TABLE 7.5

Heats of Mixing at Near Equimolar Composition
for Branched Alcohol/Alkane Systems at 25°C

	x_{alc}	ΔH Joules/mole
n-pentanol/n-hexane	.4962	482.
n-pentanol/2,2-dimethybutane	.5000	454.
n-pentanol/2,3-dimethylbutane	.4984	457.
n-pentanol/2-methylpentane	.4975	456.
n-pentanol/3-methylpentane	.4965	459.
isopentanol/n-hexane	.5068	529.
isopentanol/2,2-dimethylbutane	.4971	491.
isopentanol/2,3-dimethylbutane	.4950	494.
isopentanol/2-methylpentane	.4977	513.
isopentanol/3-methylpentane	.4972	508.
isopentanol/heptane	.4966	599.
isopentanol/octane	.4947	668.

$C_{16}H_{34}$, and found that there is very small contact energy difference between methyl and methylene groups in n-hexane/2,2-dimethylbutane system. This fact is also indicated by the heats of mixing of both n-hexane and 2,2-dimethylbutane with hepta-methylnonane which are of similar magnitude.

However, the branching effect on heats of mixing has been found to be significant in systems of n-alkane with branched alcohol (B6). The heats of mixing of branched butanol/n-hexane systems are found to decrease appreciably in the order tertiary > secondary > iso- > n-.

Thus moderate branching in an alkyl group located so as not to interfere directly with a polar groups gives rise only to second order effect, at least for the twelve alcohol/alkane systems studied, and no special modification on the model is necessary. The average root-mean-square deviation between experiment and theory (using group parameters given by equations (7.6) and (7.6)) is 8.3%. Details are given in Table 7.6. Some of the prediction results are also plotted in Figures 7.8 and 7.9.

7.4 Conclusion

The simplicity of the fundamental equation used in the model together with the quality of prediction make the analytical group solution model a very useful and powerful tool for generating heats of mixing of non-ideal systems. It

TABLE 7.6

Prediction Results on Alcohol/Alkane System at 25°C

System	RMS Deviation (%)
n-pentanol/n-hexane	5.8
n-pentanol/2,2-dimethylbutane	10.3
n-pentanol/2,3-dimethylbutane	11.8
n-pentanol/2-methylpentane	7.7
n-pentanol/3-methylpentane	9.2
isopentanol/n-hexane	9.1
isopentanol/2,2-dimethylbutane	5.9
isopentanol/2,3-dimethylbutane	5.7
isopentanol/2-methylpentane	6.0
isopentanol/3-methylpentane	5.5
isopentanol/heptane	10.6
isopentanol/octane	12.1

FIGURE 7.8

Prediction of Heats of Mixing for the System n-Pentanol/2,2-Dimethylbutane at 25°C

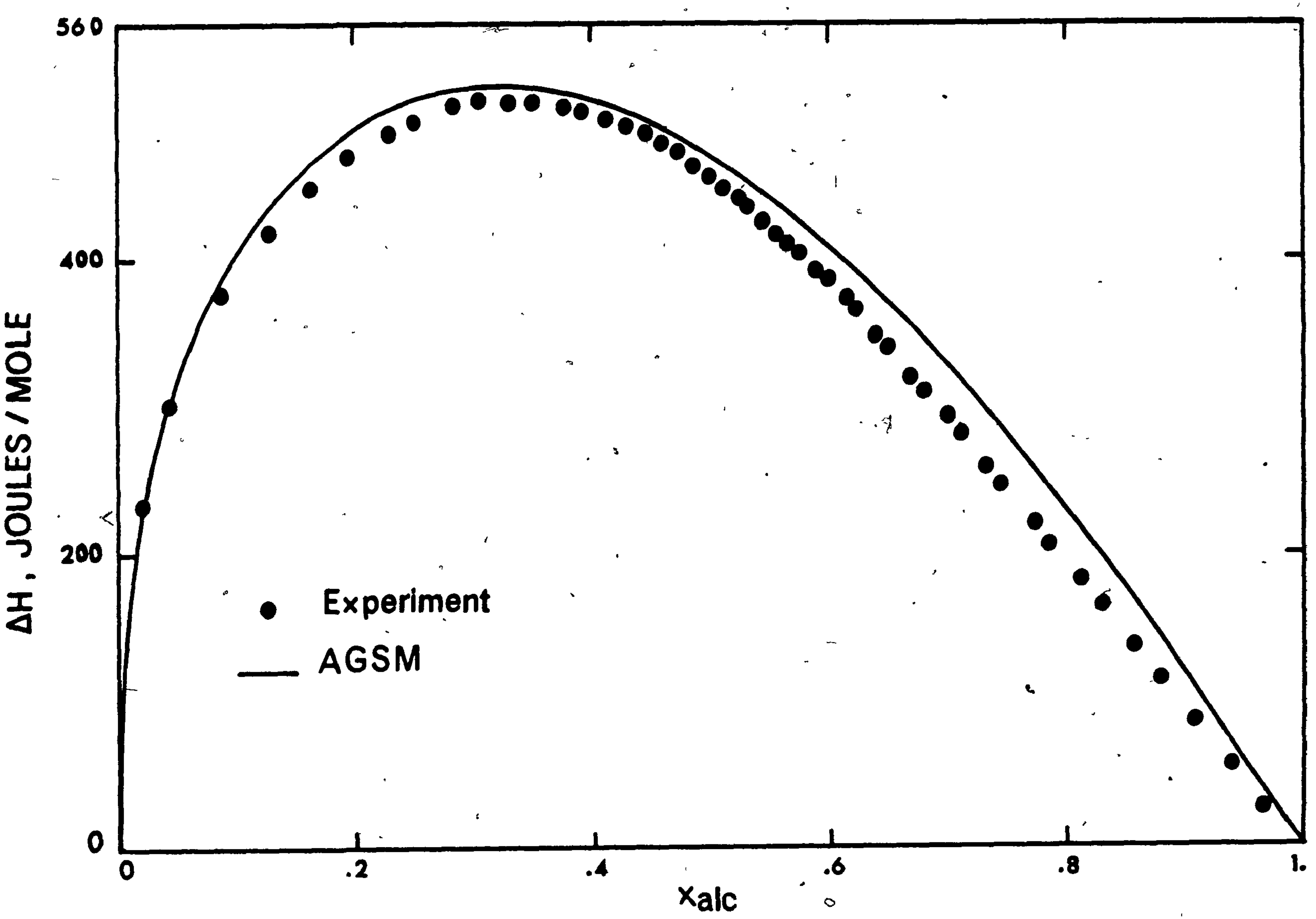
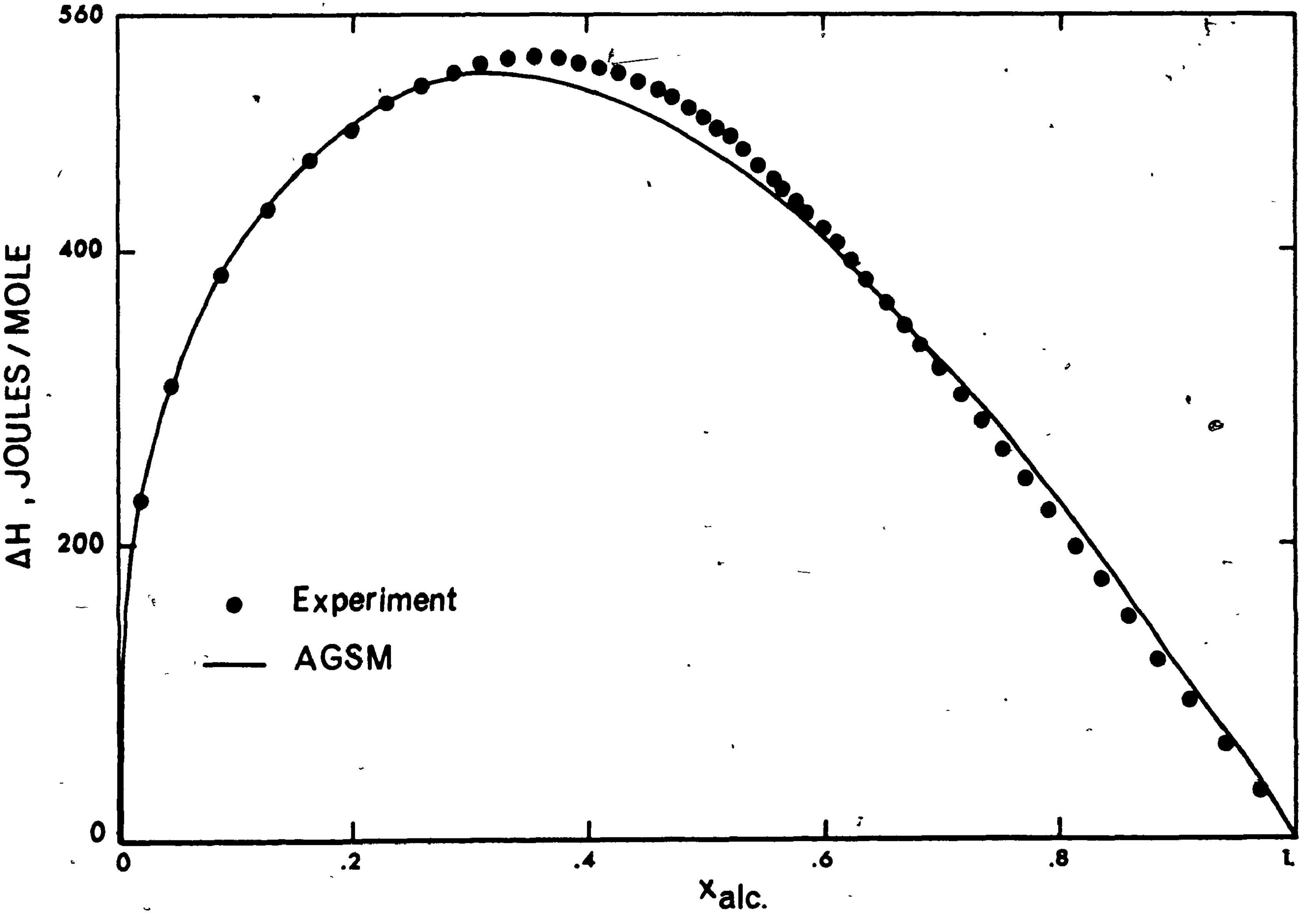

ΔH, JOULES / MOLE
560
400
200
0
0
.2
.4
.6
.8
1.
Xalc
Experiment
AGSM

FIGURE 7.9

Prediction of Heats of Mixing for the System Isopentanol/2,2-Dimethylbutane at 25°C


560
400
200
0
ΔH , JOULES / MOLE
0
.2
.4
.6
.8
1
$X_{alc.}$
● Experiment
— AGSM

has numerous advantages over the previous group solution model where the group excess enthalpies, H_k, were computed from the partial molar heats of mixing and its values were plotted graphically or fitted with polynomial functions of X_k. For a binary group system, the analytical expressions only incorporate two parameters, thereby minimizing the amount of data needed.

Moreover, the predictive analytical group solution model developed in the present study has increased the accuracy of the prediction substantially. Estimates produced by the model are generally quite adequate for preliminary process evaluation and design and very suited for computer calculation.

8. CONCLUSIONS AND RECOMMENDATIONS FOR FURTHER WORK

8.1 Apparatus and Experimental Results

A semi-continuous, isothermally operated calorimeter of the Van Ness type for measurements of endothermic heats of mixing over a wide temperature range has been constructed and thoroughly tested. The calorimeter has many desirable features. It contains no vapor space. Thus the errors associated with vaporization and condensation effects are completely eliminated.

The heats of mixing of 17 systems of n-alcohol/n-alkane and 12 systems of n-pentanol or iso-pentanol with hexane isomers over a temperature range 15°C to 55°C are believed to be a significant contribution to the body of data for the heats of mixing of binary solutions. These data are not only useful in themselves for engineering purposes but they also served as base data for the predictive model.

Some modifications can be made to the existing apparatus that would extend its capabilities.

a) The addition of other automatic burettes would extend the capabilities of the apparatus to study multicomponent mixtures. Strictly speaking, we could study multicomponent systems in the apparatus as it is by having mixtures of known compositions in the burette. Many runs would be necessary to determine the entire composition range. In the case of a ternary mixture, with one additional burette containing the third pure component, the entire composition diagram could be covered reasonably well in three consecutive runs.

b) The calorimeter can be modified to measure heats of mixing for either endothermic or exothermic systems. In addition to the existing electrical heater, a thermoelectric cooling device can be added to the present apparatus. For the measurement of an exothermic heat effect (W3), the cooling device can be adjusted to remove heat from the calorimeter.

8.2 The Predictive Model

The predictive method developed in the present study is based on the intuitive approach of treating mixtures in terms of their constituent structural groupings. The simplicity of the fundamental Wilson equation used in the model, the small amount of information required for the prediction together with the quality of prediction make the analytical group solution model a very useful and powerful tool for generating heats of mixing of non-ideal systems.

It has been shown that the group solution model for heats of mixing, put in analytical form using the Wilson equation, gives a good representation of non-ideal liquid mixtures containing the groups hydroxyl and methylene. The analytical model obviates some of the limitations and inaccuracies of the previous model and is well suited to computer calculation.

The group Wilson parameters were evaluated from experimental heats of mixing for n-alcohol/n-alkane systems in the temperature range from 15°C to 55°C. Use of these parameters regenerated experimental heats of mixing with an average accuracy of 5%. Agreement between theory and experiment was also obtained for binary systems of n-pentanol or iso-pentanol with hexane isomers. Branching in an alkyl group in these systems has only second order effect and no special means of modification on the model is necessary.

In the chemical industry, accurate design of separation operations requires reliable thermodynamic properties of mixtures. But for binary systems, the required data are often not available at the temperature and pressure where we want them, and for ternary or multicomponent mixtures, there are frequently no data at all.

The analytical group solution model is especially useful for making reliable predictions of properties of liquid mixtures. The model can be readily extended to various classes of systems containing other functional groups such as CO-, CN-... Parameters associated with pair of structural groups generated from experimental data of binary systems at various temperature can be used to project data of multigroup and multicomponent mixtures. Thus the experimental efforts could be minimized to supply the desired design data.

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APPENDICES

A1. CALCULATION OF COMPOSITION AND INTEGRAL HEATS OF MIXING

A1.1 Composition of Solution in the Dewar Flask

A1.1.1 Mass of Material Charged to Dewar Flask

Prior to, and immediately following, charging the Dewar flask, the 100 ml. stoppered volumetric flask is weighed. Since the volumetric flask is stoppered under atmospheric conditions, it contains vapour, assumed to be air at room temperature, in addition to the charged material. In order to obtain the actual amount of material placed in the Dewar flask, the mass of additional vapour in the volumetric flask must be sub-tracted from the balance weighings.

Thus

$$m_2' = m_2 - w_1' \, (\rho_{air}/\rho_1)_{T=25^{\circ}C} \qquad \text{(A1.1)}$$

and

$$w_1' = m_1 - m_2' \qquad \text{(A1.2)}$$

Solving for w_1':

$$w_1' = \frac{m_1 - m_2}{(1 - \rho_{air}/\rho_1)_{T=25^{\circ}C}} \qquad \text{(A1.3)}$$

where m_1, m_2 are initial and final weights of the stoppered volumetric flask respectively.

w_1' is the weight of pure component 1 charged to the Dewar flask.

and m_2' is defined by equations (A1.1-2).

The Dewar flask is charged quickly with the first component and is sealed immediately with the calorimetric plug. Some of the pure liquid is lost due to evaporation during this step. The small amount of liquid lost can be estimated on the assumption that the entire vapour space (total Dewar flask less liquid volume) is saturated with vapour and this vapour is completely lost.

Assuming that this vapour behaves as ideal gas, i.e. $PV = nRT$, then the mass of vapour loss, $m_{vap.}$, is

$$m_{vap.} = \frac{P_1^o V}{RT} M_1 \qquad \text{(A1.4)}$$

where P_1^o = vapour pressure of pure component 1, mm Hg

V = (Volume of Dewar flask - volume of pure liquid 1), ml

R = gas constant = 62.3×10^{-3} ml, mm Hg gmmole/^oK

T = 298^oK

M_1 = molecular weight of pure component 1

Thus, the corrected weight of pure component 1, w_1, charged to the Dewar flask is finally given by:

$$w_1 = w_1' - m_{vap.} \qquad \text{(A1.5)}$$

Al.1.2 Moles of Feed Material Injected into the Dewar Flask

The feed material is pure component 2 and the amount of material added to the Dewar flask, w_2, is calculated from:

$$w_2 = \left\{ \begin{array}{l} \text{Difference in readings of} \\ \text{burette volume} \end{array} \right\} \times \rho_2 \text{ at bath temp.}$$

where ρ_2 = density of pure component 2.

Al.1.3 Mole Fraction Component 1/2 in the Dewar Flask

Mole fraction of component 1, x_1,

$$x_1 = \frac{w_1/M_1}{w_1/M_1 + w_2/M_2} \qquad \text{(Al.6)}$$

where M_1 and M_2 are the molecular weight of pure components 1 and 2 respectively.

Mole fraction of component 2:

$$x_2 = 1 - x_1 \qquad \text{(Al.7)}$$

Al.2 Calculation of Integral Heat of Mixing at x_1

The energy of "heat" added, Q, to the system during a mixing step is given by the following equation:

$$Q = \text{(Current).(Potential Drop).(Time)} \qquad \text{(Al.8)}$$

or, referred to Figure 4.5

$$Q = \frac{e_S}{R_S} \cdot \frac{R_1 + R_2}{R_1 + R_2 + R_H} \cdot e_H \cdot \frac{R_1 + R_2}{R_1} \cdot \theta \qquad \text{(A1.9)}$$

where e_S = potential drop across the standard resistor R_S, volts

R_S = resistance of the standard resistor, ohms

R_1+R_2 = resistance of the resistors in parallel with the calorimeter heater, ohms

R_H = resistance of the calorimeter heater, ohms

e_H = potential drop across R_1, volts

θ = time of the heater operation during a mixing step, secs.

$\frac{e_S}{R_S}$ = current in the circuit

$\frac{R_1+R_2}{R_1+R_2+R_H}$ = ratio of current passing through the calorimeter heater to the total current in the circuit

$\frac{R_1+R_2}{R_1}$ = multiplication factor for the voltage divider

The integral heat of mixing is given by:

$$\Delta H(\text{Joules/Gmole}) = Q/n \qquad \text{(A1.10)}$$

where n is the number of moles of liquid in the Dewar flask,

$$n = w_1/M_1 + w_2/M_2 \qquad \text{(A1.11)}$$

A listing of the program to calculate the compositions and integral heats of mixing is given in Section A1.3.

Al.3 A Program to Compute Composition and Integral Heats of Mixing

- Listing of the Program "Heats"
- Sample of Input Data for the Program "Heats"
- Sample of Output Data for the Program "Heats"

```
C     THIS PROGRAM IS USED TO CALCULATE THE EXPERIMENTAL HEATS OF MIXING
C     OF NON IDEAL SYSTEMS
C     NPTS=NUMBER OF EXPERIMENTAL POINTS
C     RS=RESISTANCE OF STANDARD RESISTOR
C     R1= RESISTANCE OF VOLTAGE DIVIDER RESISTOR
C     R2= RESISTANCE OF VOLTAGE DIVIDER RESISTOR
C     RH=RESISTANCE OF THE HEATER
C     EH=VOLTAGE OF THE HEATER AS READ ACROSS R1
C     ES=VOLTAGE ACROSS STANDARD RESISTOR
C     W1=WEIGHT OF PURE COMPONENT INITIALLY IN DEWAR FLASK
C     AV2=V2=VOLUME OF THE OTHER PURE COMPONENT ADDED TO THE DEWAR FLASK
C     TIME=HEATING TIME
C     DELTAH=CALCULATED INTEGRAL HEATS OF MIXING
      DIMENSION TITLE1(20),TITLE2(20)
      DIMENSION AV2(50),ATIME(50),DELTAH(50),X1(50),X2(50),HX1X2(50)
      DIMENSION VEH(50),VES(50),TIME(50),Q(50)
      DIMENSION H1(50),H2(50)
      REAL M1,M2
10    READ(5,20,END=1000)TITLE1,TITLE2
   20 FORMAT(20A4/20A4)
      READ(5,15)VP1
   15 FORMAT(F10.0)
      READ(5,30)R2,R1,RH,RS
   30 FORMAT(4F10.0)
      READ(5,40)NPTS,RO1,M1,RO2,M2
   40 FORMAT(I10,4F10.0)
      READ(5,45)DW1,DW2
45    FORMAT(2F10.0)
      READ(5,50) (ATIME(I),H1(I),H2(I),VEH(I),VES(I),I=1,NPTS)
50    FORMAT(5F10.0)
C     CALCULATION OF THE CORRECTED MASS OF MATERIAL IN THE DEWAR FLASK
C
      VOLDF=325.
C     VAPORIZATION CORRECTION
      W1=(DW1-DW2)/(1.-0.0012/RO1)
      WVAP=VP1*(VOLDF-W1/RO1)*M1/0.1850E08
      W1=W1-WVAP
C     CALCULATION OF INTEGRAL HEATS OF MIXING
      V2=0.
      TIME(1)=ATIME(1)
      DO 70 I=2,NPTS
70    TIME(I)=ATIME(I)-ATIME(I-1)
      DO 100 I=1,NPTS
      AV2(I)=H2(I)-H1(I)
      V2=V2+AV2(I)
      RAT1=W1/M1
      RAT2=RO2*V2/M2
      DQ=(VES(I)/RS)*((R1+R2)/(R1+R2+RH))*VEH(I)*((R1+R2)/R1)*TIME(I)
      IF(I.EQ.1) GO TO 80
      Q(I)=Q(I-1)+DQ
      GO TO 90
80    Q(I)=DQ
90    HEATS=Q(I)/(RAT1+RAT2)
      DELTAH(I)=HEATS
```

```
C       CALCULATION OF COMPOSITION
        X1(I)=RAT1/(RAT1+RAT2)
        X2(I)=1.-X1(I)
        HX1X2(I)=DELTAH(I)/(X1(I)*X2(I))
 100    CONTINUE
        PRINT 180
 180    FORMAT(1H1)
        PRINT 190,TITLE1,TITLE2
 190    FORMAT(20A4/20A4)
        PRINT 209,DW1,DW2,RO1,M1,RO2,M2
209     FORMAT(T5,'DW1=',F10.4,T25,'DW2=',F10.4/T5,'RO1=',F10.4,T25,'M1='
       1,F10.4,T45,'RO2=',F10.4,T65,'M2=',F10.4/)
        PRINT210
210     FORMAT(T10,'N',T15,'TIME',T27,'VOL.',T42,'VEH',T57,'VES',T67,'X1',
       1T77,'X2',T87,'DELTAH',T95,'DELTAH/X1X2'/)
        PRINT 220, (I,ATIME(I),AV2(I),VEH(I),VES(I),X1(I),X2(I),DELTAH(I),
       1HX1X2(I),I=1,NPTS)
220     FORMAT(5X,I5,2F10.2,F15.5,F15.6,2F10.4,2F10.1 )
         WRITE(7,20)TITLE1,TITLE2
        DO 230 I=1,NPTS
230     WRITE(7,240)X2(I),DELTAH(I),HX1X2(I)
240     FORMAT(F20.4,2F20.1)
        GO TO 10
1000    STOP
        END

 EFFECT*  ID,EBCDIC,SOURCE,NOLIST,NODECK,LOAD,NOMAP
 EFFECT*  NAME = MAIN    , LINECNT =       56
*    SOURCE STATEMENTS =        58,PROGRAM SIZE =      4364
*   NO DIAGNOSTICS GENERATED
```

```
SAMPLE INPUT DATA FOR 'HEATS'

HEAT OF MIXING OF ISOPENTANOL - N-HEPTANE AT 25 DEG C  JUNE 19 1973
FIRST COMPONENT - N-HEPTANE THERMISTOR  READING-103700
VP1= 52.25
R2= 2700.   R1= 300.   RH= 45.   RS=0.99999
PTS= 26   RO1=0.6795   M1= 100.206   RO2=0.8099   M2= 88.150
DW1= 123.89607   DW2= 57.41060

    N        TIME        H1        H2       VEH       VES
    1       704.70      0.25      1.86    0.31654   0.07796
    2      1016.80      4.86      4.14    0.31654   0.07796
    3      1334.90      0.20      4.11    0.31654   0.07796
    4      1572.40      0.21      4.16    0.31654   0.07796
    5      1775.30      0.21      4.19    0.31654   0.07796
    6      1955.80      0.21      4.19    0.31654   0.07796
    7      2117.40      0.20      4.20    0.31654   0.07796
    8      2263.90      0.20      4.13    0.31654   0.07796
    9      2397.40      0.21      4.13    0.31654   0.07796
   10      2519.70      0.21      4.17    0.31654   0.07796
   11      2628.40      0.20      4.13    0.31654   0.07796
   12      2733.40      0.22      4.29    0.31654   0.07796
   13      2828.95      0.20      4.15    0.31654   0.07796
   14      2914.70      0.21      4.22    0.31654   0.07796
   15      2994.20      0.22      4.23    0.31654   0.07796
   16      3068.00      0.21      4.22    0.31654   0.07796
   17      3135.50      0.21      4.31    0.31654   0.07796
   18      3197.40      0.21      4.27    0.31654   0.07796
   19      3252.40      0.21      4.24    0.31654   0.07796
   20      3302.60      0.20      4.21    0.31654   0.07796
   21      3349.95      0.21      4.12    0.31654   0.07796
   22      3391.20      0.19      4.18    0.31654   0.07796
   23      3435.90      0.20      4.25    0.31654   0.07796
   24      3467.70      0.21      4.18    0.31654   0.07796
   25      3498.00      0.19      4.15    0.31654   0.07796
   26      3530.20      0.21      4.07    0.31654   0.07796
```

SAMPLE OF OUTPUT DATA FOR THE PROGRAM 'HEATS'

```
HEAT OF MIXING OF ISOPENTANOL- N-HEPTANE AT 25 DEG C  JUNE 19 1973
FIRST COMPONENT - N-HEPTANE THERMISTOR READING-103700
   DW1=  123.8941        DW2=    57.4106
   RO1=     0.6795       M1=  100.2060        RO2=     0.8059       M2=    88.1500

       N    TIME          VOL.          VEH          VES         X1        X2        DELTAH  DELTAH/X1

       1     704.70       1.61        0.31654     0.077960    0.9783    0.0217     252.4   11898.2
       2    1016.80       2.28        0.31654     0.077960    0.9492    0.0508     353.4    7323.6
       3    1334.90       3.93        0.31654     0.077960    0.9027    0.0973     441.2    5025.5
       4    1572.40       3.95        0.31654     0.077960    0.8605    0.1395     495.4    4127.0
       5    1775.30       3.98        0.31654     0.077960    0.8217    0.1783     534.2    3646.7
       6    1955.80       3.98        0.31654     0.077960    0.7863    0.2137     563.1    3351.7
       7    2117.40       4.00        0.31654     0.077960    0.7537    0.2463     584.3    3147.7
       8    2263.90       3.93        0.31654     0.077960    0.7242    0.2758     600.3    3005.2
       9    2397.40       3.91        0.31654     0.077960    0.6970    0.3030     611.8    2896.7
      10    2519.70       3.96        0.31654     0.077960    0.6714    0.3286     619.4    2807.8
      11    2628.40       3.84        0.31654     0.077960    0.6484    0.3516     624.0    2736.9
      12    2733.40       4.07        0.31654     0.077960    0.6256    0.3744     626.1    2673.3
      13    2828.95       3.95        0.31654     0.077960    0.6050    0.3950     626.7    2622.5
      14    2914.70       4.01        0.31654     0.077960    0.5855    0.4145     624.8    2574.5
      15    2994.20       4.01        0.31654     0.077960    0.5671    0.4329     621.8    2532.8
      16    3068.00       4.01        0.31654     0.077960    0.5499    0.4501     617.8    2495.9
      17    3135.50       4.10        0.31654     0.077960    0.5334    0.4666     612.3    2460.3
      18    3197.40       4.06        0.31654     0.077960    0.5179    0.4821     606.3    2428.5
      19    3252.40       4.03        0.31654     0.077960    0.5034    0.4966     599.5    2398.3
      20    3302.60       4.06        0.31654     0.077960    0.4896    0.5104     592.1    2369.5
      21    3349.95       3.91        0.31654     0.077960    0.4771    0.5229     585.2    2345.7
      22    3391.20       3.99        0.31654     0.077960    0.4649    0.5351     577.2    2320.4
      23    3435.90       4.05        0.31654     0.077960    0.4531    0.5469     570.1    2300.5
      24    3467.70       3.97        0.31654     0.077960    0.4422    0.5578     561.4    2276.2
      25    3498.00       3.96        0.31654     0.077960    0.4318    0.5682     553.0    2254.0
      26    3530.20       3.86        0.31654     0.077960    0.4221    0.5779     545.6    2236.7
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A2. Tabulated Experimental Results

- Heats of Mixing for the System Benzene/Cyclohexane at 25°C and 55°C
- Heats of Mixing for Alcohol/Alkane Systems

TABLE A1

HEATS OF MIXING AT 25 DEG.C FOR THE SYSTEM BENZENE/CYCLOHEXANE
X=MOLE FRACTION OF BENZENE, DELTA H=HEATS OF MIXING

N	X	DELTA H	DEL H/X1X2
1	0.0468	139.0	3115.
2	0.0992	278.4	3115.
3	0.1508	399.4	3119.
4	0.1969	493.8	3123.
5	0.2272	549.2	3128.
6	0.2781	629.2	3134.
7	0.3006	660.2	3140.
8	0.3291	694.4	3145.
9	0.3684	733.2	3151.
10	0.3896	751.2	3159.
11	0.4247	773.5	3166.
12	0.4551	786.6	3172.
13	0.4808	793.3	3178.
14	0.5002	796.2	3185.
15	0.5192	796.6	3191.
16	0.5303	795.3	3193.
17	0.5382	794.6	3197.
18	0.5470	792.9	3200.
19	0.5479	793.6	3204.
20	0.5744	784.7	3210.
21	0.5847	780.9	3216.
22	0.6023	771.8	3222.
23	0.6208	760.6	3231.
24	0.6404	746.1	3240.
25	0.6699	698.1	3157.
26	0.6904	676.5	3165.
27	0.7104	653.4	3176.
28	0.7305	646.7	3285.
29	0.7470	623.3	3298.
30	0.7831	564.1	3321.
31	0.8089	517.4	3347.
32	0.8582	411.1	3378.
33	0.8089	528.8	3421.
34	0.9402	193.7	3445.
35	0.9845	53.2	3487.

TABLE A2

HEATS OF MIXING AT 50 DEG.C FOR THE SYSTEM BENZENE/CYCLOHEXANE
X=MOLE FRACTION OF BENZENE, DELTA H=HEATS OF MIXING

N	X	DELTA H	DEL H/X1X2
1	0.0487	131.4	2837.
2	0.0922	237.8	2841.
3	0.1315	324.7	2843.
4	0.1685	398.9	2847.
5	0.2025	460.6	2852.
6	0.2341	511.5	2853.
7	0.2633	554.2	2857.
8	0.2903	589.2	2860.
9	0.3200	623.0	2863.
10	0.3430	646.3	2868.
11	0.3813	677.1	2870.
12	0.4011	690.6	2875.
13	0.4197	701.4	2880.
14	0.4533	714.7	2884.
15	0.4684	720.1	2892.
16	0.4969	724.9	2898.
17	0.5097	725.7	2904.
18	0.5108	726.7	2908.
19	0.5449	722.1	2912.
20	0.5279	724.7	2908.
21	0.5655	717.0	2918.
22	0.5713	714.2	2916.
23	0.5822	711.2	2924.
24	0.6077	699.2	2933.
25	0.6211	691.4	2938.
26	0.6357	681.8	2944.
27	0.6509	670.3	2950.
28	0.6668	657.4	2959.
29	0.7017	621.3	2968.
30	0.7305	586.1	2977.
31	0.7501	559.9	2987.
32	0.7691	531.9	2995.
33	0.8001	481.3	3009.
34	0.8304	426.5	3028.
35	0.8520	383.3	3040.
36	0.8820	318.3	3058.
37	0.9012	274.1	3078.
38	0.9404	173.7	3100.
39	0.9703	90.1	3125.

TABLE A3

HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-BUTANOL+N-HEXANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0272	193.8	7324.0
2	0.0546	257.0	4978.0
3	0.1044	328.4	3512.0
4	0.1479	371.8	2950.0
5	0.1883	402.4	2633.0
6	0.2252	423.8	2429.0
7	0.2582	438.0	2287.0
8	0.2904	446.1	2165.0
9	0.3198	450.3	2070.0
10	0.3478	450.9	1988.0
11	0.3730	448.3	1917.0
12	0.3997	442.7	1845.0
13	0.4203	437.8	1797.0
14	0.4379	432.0	1755.0
15	0.4552	425.3	1715.0
16	0.4727	418.0	1677.0
17	0.4881	410.8	1644.0
18	0.5038	403.0	1612.0
19	0.5207	393.6	1577.0
20	0.5338	386.5	1553.0
21	0.5460	379.0	1529.0
22	0.5559	373.0	1511.0
23	0.5670	365.8	1490.0
24	0.5730	363.1	1484.0
25	0.5767	359.8	1474.0
26	0.5828	356.4	1466.0
27	0.5866	353.1	1456.0
28	0.5927	349.6	1448.0
29	0.5956	347.1	1441.0
30	0.6026	342.2	1429.0
31	0.6130	335.0	1412.0
32	0.6241	327.3	1395.0
33	0.6361	319.2	1379.0
34	0.6479	310.7	1362.0
35	0.6605	301.6	1345.0
36	0.6736	291.8	1327.0
37	0.6870	281.5	1309.0
38	0.7011	270.3	1290.0
39	0.7159	258.9	1273.0
40	0.7313	246.6	1255.0
41	0.7465	233.5	1234.0
42	0.7624	219.0	1214.0
43	0.7797	205.8	1198.0
44	0.7975	190.7	1181.0
45	0.8151	176.2	1169.0
46	0.8338	159.6	1152.0
47	0.8549	141.5	1141.0
48	0.8766	122.2	1130.0
49	0.8990	102.3	1127.0
50	0.9227	81.3	1140.0
51	0.9472	58.5	1170.0
52	0.9729	34.4	1304.0

TABLE A4:

HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-BUTANOL+N-HEPTANE.
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0337	203.1	6238.0
2	0.0631	266.7	4511.0
3	0.1213	349.2	3276.0
4	0.1720	399.6	2806.0
5	0.2202	435.6	2537.0
6	0.2614	457.6	2370.0
7	0.2984	471.5	2252.0
8	0.3326	478.1	2154.0
9	0.3630	480.3	2077.0
10	0.3911	479.1	2012.0
11	0.4175	474.5	1951.0
12	0.4405	469.5	1905.0
13	0.4656	461.1	1853.0
14	0.4857	453.9	1817.0
15	0.5043	445.5	1782.0
16	0.5204	438.0	1755.0
17	0.5359	429.8	1728.0
18	0.5508	421.4	1703.0
19	0.5650	413.1	1681.0
20	0.5779	405.2	1661.0
21	0.5904	397.8	1645.0
22	0.5935	393.3	1630.0
23	0.6018	389.6	1626.0
24	0.6020	387.2	1616.0
25	0.6118	380.5	1602.0
26	0.6215	375.7	1597.0
27	0.6125	381.9	1609.0
28	0.6219	372.5	1584.0
29	0.6315	369.1	1586.0
30	0.6323	364.8	1569.0
31	0.6410	362.4	1575.0
32	0.6428	356.6	1553.0
33	0.6487	356.0	1562.0
34	0.6539	348.8	1541.0
35	0.6651	340.1	1527.0
36	0.6772	330.1	1510.0
37	0.6895	319.8	1494.0
38	0.7019	309.0	1477.0
39	0.7156	296.5	1457.0
40	0.7295	284.9	1444.0
41	0.7437	272.2	1428.0
42	0.7585	257.5	1406.0
43	0.7743	242.6	1388.0
44	0.7907	227.1	1372.0
45	0.8075	211.1	1358.0
46	0.8237	194.6	1340.0
47	0.8416	175.8	1319.0
48	0.8613	156.4	1309.0
49	0.8811	134.6	1285.0
50	0.9019	111.7	1263.0
51	0.9229	88.0	1237.0
52	0.9456	62.6	1217.0
53	0.9749	27.1	1109.0

TABLE A5:

HEATS OF MIXING AT 15 DEG. C FOR THE SYSTEM N-BUTANOL + N-OCTANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0352	252.3	7429.0
2	0.0680	324.2	5116.0
3	0.1266	405.8	3670.0
4	0.1787	457.5	3117.0
5	0.2265	492.3	2810.0
6	0.2687	513.8	2615.0
7	0.3074	527.4	2477.0
8	0.3430	534.1	2370.0
9	0.3749	535.7	2286.0
10	0.4030	533.9	2219.0
11	0.4286	529.2	2161.0
12	0.4531	522.9	2110.0
13	0.4745	516.2	2070.0
14	0.4950	507.7	2031.0
15	0.5128	499.2	1998.0
16	0.5300	490.2	1968.0
17	0.5442	482.0	1943.0
18	0.5580	473.8	1921.0
19	0.5718	465.2	1900.0
20	0.5844	456.6	1880.0
21	0.5969	448.3	1863.0
22	0.6092	439.0	1844.0
23	0.6122	439.4	1851.0
24	0.6206	430.2	1827.0
25	0.6212	433.0	1840.0
26	0.6304	425.9	1828.0
27	0.6310	422.1	1813.0
28	0.6399	418.0	1814.0
29	0.6412	413.9	1799.0
30	0.6496	409.7	1800.0
31	0.6512	405.4	1785.0
32	0.6602	400.7	1786.0
33	0.6709	391.5	1773.0
34	0.6823	380.6	1756.0
35	0.6944	369.9	1743.0
36	0.7061	359.4	1732.0
37	0.7189	347.0	1717.0
38	0.7323	333.7	1702.0
39	0.7454	320.3	1688.0
40	0.7593	306.1	1675.0
41	0.7735	291.2	1662.0
42	0.7887	274.8	1649.0
43	0.8045	256.5	1631.0
44	0.8212	238.6	1625.0
45	0.8373	219.5	1611.0
46	0.8547	198.5	1598.0
47	0.8728	176.1	1586.0
48	0.8921	151.6	1575.0
49	0.9123	124.9	1561.0
50	0.9335	96.8	1559.0
51	0.9558	65.9	1561.0
52	0.9782	33.0	1546.0

TABLE A6:

HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-BUTANOL+N-DECANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0469	275.8	6171.0
2	0.0766	345.6	4886.0
3	0.1428	448.0	3660.0
4	0.2014	509.4	3167.0
5	0.2531	551.1	2915.0
6	0.2985	577.3	2757.0
7	0.3399	591.7	2637.0
8	0.3756	599.9	2558.0
9	0.4092	601.2	2487.0
10	0.4399	599.2	2432.0
11	0.4661	593.8	2386.0
12	0.4890	587.0	2349.0
13	0.5079	580.9	2324.0
14	0.5279	572.2	2296.0
15	0.5455	563.8	2274.0
16	0.5635	554.2	2253.0
17	0.5821	542.5	2230.0
18	0.5970	533.1	2216.0
19	0.6107	523.3	2201.0
20	0.6225	514.4	2189.0
21	0.6341	505.1	2177.0
22	0.6450	496.2	2167.0
23	0.6551	487.4	2157.0
24	0.6653	479.0	2151.0
25	0.6668	487.7	2195.0
26	0.6748	470.5	2144.0
27	0.6754	479.9	2189.0
28	0.6835	462.3	2137.0
29	0.6840	471.6	2182.0
30	0.6933	462.3	2174.0
31	0.7026	452.2	2164.0
32	0.7123	441.6	2155.0
33	0.7227	430.7	2149.0
34	0.7329	418.9	2140.0
35	0.7431	407.2	2133.0
36	0.7542	395.0	2131.0
37	0.7650	381.7	2123.0
38	0.7759	368.6	2120.0
39	0.7879	352.8	2111.0
40	0.8001	337.3	2109.0
41	0.8125	321.0	2107.0
42	0.8257	302.8	2104.0
43	0.8394	283.4	2102.0
44	0.8531	262.9	2098.0
45	0.8684	240.2	2102.0
46	0.8831	217.5	2107.0
47	0.8980	192.4	2100.0
48	0.9140	165.4	2104.0
49	0.9298	137.8	2111.0
50	0.9468	106.5	2114.0
51	0.9645	72.3	2112.0
52	0.9816	38.3	2119.0

TABLE A7:

HEATS OF MIXING AT 15 DEG. C FOR THE SYSTEM N-PENTANOL+N-HEPTANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0315	215.2	7055.0
2	0.0518	261.9	5333.0
3	0.1002	330.4	3665.0
4	0.1435	373.0	3035.0
5	0.1835	403.5	2693.0
6	0.2204	425.4	2476.0
7	0.2542	441.9	2331.0
8	0.2052	362.2	2221.0
9	0.3140	459.9	2135.0
10	0.3384	463.4	2070.0
11	0.3619	465.8	2017.0
12	0.3833	463.3	1960.0
13	0.4019	461.0	1918.0
14	0.4211	457.8	1878.0
15	0.4400	452.9	1838.0
16	0.4568	447.4	1803.0
17	0.4739	440.5	1767.0
18	0.4883	434.0	1737.0
19	0.5054	426.2	1705.0
20	0.5172	419.8	1681.0
21	0.5284	413.7	1660.0
22	0.5407	407.0	1639.0
23	0.5525	400.0	1618.0
24	0.5570	399.7	1620.0
25	0.5639	393.2	1599.0
26	0.5668	393.4	1602.0
27	0.5747	386.4	1581.0
28	0.5769	386.4	1583.0
29	0.5849	379.2	1562.0
30	0.5877	378.5	1562.0
31	0.5986	370.5	1542.0
32	0.6102	361.8	1521.0
33	0.6222	352.8	1501.0
34	0.6341	343.4	1480.0
35	0.6472	333.1	1459.0
36	0.6605	321.8	1435.0
37	0.6739	310.3	1412.0
38	0.6882	298.3	1390.0
39	0.7027	285.6	1367.0
40	0.7179	272.0	1343.0
41	0.7334	257.7	1318.0
42	0.7504	241.8	1291.0
43	0.7679	225.8	1267.0
44	0.7867	207.6	1237.0
45	0.8063	189.6	1214.0
46	0.8269	169.0	1181.0
47	0.8485	148.3	1154.0
48	0.8704	127.0	1126.0
49	0.8941	102.9	1087.0
50	0.9162	81.1	1056.0
51	0.9424	54.3	1001.0
52	0.9722	25.3	935.0

TABLE A8:

HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-PENTANOL+N-DECANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0418	285.8	7135.0
2	0.0665	338.8	5458.0
3	0.1265	427.7	3871.0
4	0.1804	482.3	3262.0
5	0.2293	518.3	2933.0
6	0.2717	545.0	2754.0
7	0.3104	563.0	2630.0
8	0.3445	574.9	2546.0
9	0.3758	581.5	2479.0
10	0.4047	584.0	2424.0
11	0.4307	583.6	2380.0
12	0.4546	580.4	2341.0
13	0.4754	575.4	2307.0
14	0.4951	569.7	2279.0
15	0.5140	561.8	2249.0
16	0.5306	553.7	2223.0
17	0.5448	546.3	2203.0
18	0.5586	539.0	2186.0
19	0.5733	530.1	2167.0
20	0.5866	521.1	2149.0
21	0.5989	511.9	2131.0
22	0.6100	503.4	2116.0
23	0.6209	494.5	2101.0
24	0.6291	481.4	2063.0
25	0.6309	486.0	2087.0
26	0.6354	476.8	2058.0
27	0.6407	477.2	2073.0
28	0.6434	470.1	2049.0
29	0.6489	451.8	1983.0
30	0.6527	460.8	2033.0
31	0.6646	450.9	2023.0
32	0.6750	441.6	2013.0
33	0.6859	430.7	1999.0
34	0.6964	420.1	1987.0
35	0.7077	408.5	1975.0
36	0.7198	395.7	1962.0
37	0.7318	382.9	1951.0
38	0.7440	368.7	1936.0
39	0.7572	353.7	1924.0
40	0.7709	337.5	1911.0
41	0.7845	321.0	1899.0
42	0.7983	302.9	1881.0
43	0.8128	284.7	1871.0
44	0.8284	263.6	1854.0
45	0.8450	240.7	1838.0
46	0.8616	218.6	1833.0
47	0.8787	194.0	1820.0
48	0.8979	165.6	1806.0
49	0.9174	135.1	1783.0
50	0.9372	103.1	1751.0
51	0.9570	71.8	1745.0
52	0.9783	36.4	1713.0

TABLE A9:

HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-HEXANOL+N-HEPTANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0280	210.8	7746.0
2	0.0455	248.5	5723.0
3	0.0885	307.6	3813.0
4	0.1276	343.8	3088.0
5	0.1642	369.3	2691.0
6	0.1961	387.8	2460.0
7	0.2260	402.8	2303.0
8	0.2531	412.5	2182.0
9	0.2773	420.2	2097.0
10	0.3008	426.3	2027.0
11	0.3231	430.2	1967.0
12	0.3438	432.5	1917.0
13	0.3632	433.2	1873.0
14	0.3812	432.6	1834.0
15	0.3997	431.2	1797.0
16	0.4169	429.3	1766.0
17	0.4360	426.2	1733.0
18	0.4519	421.3	1701.0
19	0.4659	416.8	1675.0
20	0.4789	411.8	1650.0
21	0.4908	406.9	1628.0
22	0.5017	402.2	1609.0
23	0.5139	396.9	1589.0
24	0.5216	390.3	1564.0
25	0.5256	391.7	1571.0
26	0.5318	384.7	1545.0
27	0.5366	386.4	1554.0
28	0.5416	379.1	1527.0
29	0.5488	379.1	1531.0
30	0.5527	373.1	1509.0
31	0.5640	366.2	1489.0
32	0.5763	358.0	1466.0
33	0.5887	349.9	1445.0
34	0.6012	341.2	1423.0
35	0.6145	331.6	1400.0
36	0.6284	322.0	1379.0
37	0.6418	311.7	1356.0
38	0.6567	299.8	1330.0
39	0.6731	286.7	1303.0
40	0.6890	274.1	1279.0
41	0.7067	258.5	1247.0
42	0.7255	241.6	1213.0
43	0.7446	244.0	1283.0
44	0.7647	206.9	1150.0
45	0.7863	188.2	1120.0
46	0.8049	171.5	1092.0
47	0.8287	149.5	1053.0
48	0.8536	126.6	1013.0
49	0.8792	102.9	969.0
50	0.9070	77.2	915.0
51	0.9354	52.7	872.0
52	0.9636	26.8	764.0

TABLE A10:

HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-HEXANOL+N-OCTANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0232	203.8	8991.0
2	0.0503	270.9	5671.0
3	0.0977	337.6	3830.0
4	0.1409	377.9	3122.0
5	0.1795	406.1	2757.0
6	0.2164	427.8	2523.0
7	0.2493	443.7	2371.0
8	0.2797	454.9	2258.0
9	0.3080	462.5	2170.0
10	0.3318	466.3	2103.0
11	0.3529	468.1	2050.0
12	0.3746	470.2	2007.0
13	0.3953	470.2	1967.0
14	0.4152	468.6	1930.0
15	0.4337	465.7	1896.0
16	0.4503	462.4	1868.0
17	0.4666	457.7	1839.0
18	0.4810	452.8	1814.0
19	0.4945	447.7	1791.0
20	0.5067	442.4	1770.0
21	0.5177	437.2	1751.0
22	0.5287	432.3	1735.0
23	0.5404	426.4	1717.0
24	0.5497	419.1	1693.0
25	0.5516	420.7	1701.0
26	0.5593	414.3	1681.0
27	0.5642	413.1	1680.0
28	0.5694	407.5	1662.0
29	0.5748	406.4	1663.0
30	0.5798	400.8	1645.0
31	0.5914	392.4	1624.0
32	0.6028	385.0	1608.0
33	0.6142	376.5	1589.0
34	0.6261	367.1	1568.0
35	0.6386	357.5	1549.0
36	0.6517	346.6	1527.0
37	0.6648	334.9	1503.0
38	0.6793	322.9	1482.0
39	0.6945	309.8	1460.0
40	0.7098	294.8	1431.0
41	0.7250	280.5	1407.0
42	0.7421	264.1	1380.0
43	0.7593	247.8	1356.0
44	0.7783	229.1	1328.0
45	0.7973	209.1	1294.0
46	0.8187	186.7	1258.0
47	0.8387	166.0	1227.0
48	0.8623	141.4	1191.0
49	0.8867	115.4	1149.0
50	0.9114	89.8	1112.0
51	0.9397	59.9	1057.0
52	0.9681	29.3	949.0

TABLE A11:

HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-OCTANOL+N-HEXANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0171	160.7	9563.0
2	0.0316	199.0	6504.0
3	0.0627	244.2	4156.0
4	0.0925	271.7	3237.0
5	0.1185	289.6	2772.0
6	0.1431	303.6	2476.0
7	0.1679	315.5	2258.0
8	0.1923	325.2	2094.0
9	0.2144	331.8	1970.0
10	0.2334	336.9	1883.0
11	0.2513	341.1	1813.0
12	0.2690	344.9	1754.0
13	0.2861	347.2	1700.0
14	0.3014	349.3	1659.0
15	0.3165	350.9	1622.0
16	0.3321	351.8	1586.0
17	0.3474	352.1	1553.0
18	0.3619	351.7	1523.0
19	0.3753	351.2	1498.0
20	0.3880	350.2	1475.0
21	0.4012	348.6	1451.0
22	0.4128	346.6	1430.0
23	0.4239	344.3	1410.0
24	0.4342	342.2	1393.0
25	0.4446	339.8	1376.0
26	0.4523	337.6	1363.0
27	0.4628	326.2	1312.0
28	0.4719	324.7	1303.0
29	0.4820	322.3	1291.0
30	0.4924	318.7	1275.0
31	0.5033	315.2	1261.0
32	0.5156	310.4	1243.0
33	0.5280	305.8	1227.0
34	0.5410	300.0	1208.0
35	0.5547	293.9	1190.0
36	0.5682	287.8	1173.0
37	0.5832	280.3	1153.0
38	0.5995	271.1	1129.0
39	0.6166	260.3	1101.0
40	0.6344	251.0	1082.0
41	0.6534	239.2	1056.0
42	0.6726	227.0	1031.0
43	0.6931	213.1	1002.0
44	0.7151	198.2	973.0
45	0.7379	182.2	942.0
46	0.7627	164.9	911.0
47	0.7896	144.7	871.0
48	0.8182	124.5	837.0
49	0.8494	102.0	797.0
50	0.8831	76.9	745.0
51	0.9198	50.6	686.0
52	0.9564	24.9	598.0

TABLE A12:

HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-OCTANOL+N-HEPTANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0208	188.3	9247.0
2	0.0352	224.4	6608.0
3	0.0699	276.4	4252.0
4	0.1017	307.2	3363.0
5	0.1316	328.3	2873.0
6	0.1598	344.3	2564.0
7	0.1854	355.8	2356.0
8	0.2076	363.9	2212.0
9	0.2278	370.8	2108.0
10	0.2484	376.6	2017.0
11	0.2686	381.5	1942.0
12	0.2883	385.3	1878.0
13	0.3063	388.0	1826.0
14	0.3234	389.9	1782.0
15	0.3383	390.6	1745.0
16	0.3532	390.9	1711.0
17	0.3675	391.4	1684.0
18	0.3823	390.8	1655.0
19	0.3960	389.9	1630.0
20	0.4094	388.6	1607.0
21	0.4223	386.4	1584.0
22	0.4341	384.5	1565.0
23	0.4450	382.1	1547.0
24	0.4553	379.9	1532.0
25	0.4583	382.6	1541.0
26	0.4665	376.3	1512.0
27	0.4678	380.9	1530.0
28	0.4750	373.6	1498.0
29	0.4778	378.3	1516.0
30	0.4880	373.8	1496.0
31	0.5012	370.5	1482.0
32	0.5136	366.2	1466.0
33	0.5263	360.3	1445.0
34	0.5392	354.8	1428.0
35	0.5528	348.6	1410.0
36	0.5673	341.0	1389.0
37	0.5816	333.1	1369.0
38	0.5978	323.6	1346.0
39	0.6150	313.5	1324.0
40	0.6326	301.7	1298.0
41	0.6503	290.6	1278.0
42	0.6698	277.1	1253.0
43	0.6913	261.6	1226.0
44	0.7147	243.3	1193.0
45	0.7395	224.8	1167.0
46	0.7656	188.1	1048.0
47	0.7941	164.3	1005.0
48	0.8242	140.3	968.0
49	0.8547	114.9	925.0
50	0.8869	87.9	876.0
51	0.9244	57.7	825.0
52	0.9581	28.9	720.0

TABLE A13:

HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-OCTANOL+N-OCTANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0201	192.3	9762.0
2	0.0378	241.7	6646.0
3	0.0741	297.1	4331.0
4	0.1096	332.3	3405.0
5	0.1418	355.1	2918.0
6	0.1705	371.4	2626.0
7	0.1966	382.6	2422.0
8	0.2205	391.9	2280.0
9	0.2437	399.6	2168.0
10	0.2661	405.8	2078.0
11	0.2872	410.7	2006.0
12	0.3068	414.7	1950.0
13	0.3262	417.2	1898.0
14	0.3437	418.4	1855.0
15	0.3607	418.3	1814.0
16	0.3757	418.0	1782.0
17	0.3905	417.7	1755.0
18	0.4048	416.8	1730.0
19	0.4197	415.5	1706.0
20	0.4336	413.6	1684.0
21	0.4470	411.3	1664.0
22	0.4618	407.1	1638.0
23	0.4723	404.3	1622.0
24	0.4837	400.8	1605.0
25	0.4909	396.6	1587.0
26	0.4942	397.4	1590.0
27	0.500[illegible]	393.7	1575.0
28	0.5048	393.0	1572.0
29	0.5099	390.6	1563.0
30	0.5203	386.6	1549.0
31	0.5308	381.8	1533.0
32	0.5420	376.6	1517.0
33	0.5536	370.7	1500.0
34	0.5664	364.2	1483.0
35	0.5793	356.8	1464.0
36	0.5936	348.8	1446.0
37	0.6081	339.8	1426.0
38	0.6239	329.4	1404.0
39	0.6405	317.3	1378.0
40	0.6586	304.2	1353.0
41	0.6767	289.9	1325.0
42	0.6964	273.8	1295.0
43	0.7177	256.1	1264.0
44	0.7391	237.6	1232.0
45	0.7620	217.4	1199.0
46	0.7848	196.9	1166.0
47	0.8077	175.4	1129.0
48	0.8352	150.1	1090.6
49	0.8638	123.8	1052.0
50	0.8945	95.1	1008.0
51	0.9289	63.1	955.0
52	0.9609	33.0	879.0

TABLE A14:

HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-OCTANOL+N-DECANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0234	221.6	9695.0
2	0.0447	278.5	6521.0
3	0.0891	346.2	4265.0
4	0.1298	385.4	3412.0
5	0.1654	410.3	2972.0
6	0.1981	429.2	2702.0
7	0.2261	440.9	2520.0
8	0.2532	452.3	2392.0
9	0.2803	460.2	2281.0
10	0.3056	466.9	2200.0
11	0.3282	471.0	2136.0
12	0.3494	474.0	2085.0
13	0.3701	474.6	2036.0
14	0.3884	475.3	2001.0
15	0.4062	475.2	1970.0
16	0.4235	473.9	1941.0
17	0.4400	472.1	1916.0
18	0.4559	469.6	1893.0
19	0.4707	466.1	1871.0
20	0.4841	463.0	1854.0
21	0.4968	459.7	1839.0
22	0.5095	455.3	1822.0
23	0.5213	450.9	1807.0
24	0.5322	446.9	1795.0
25	0.5428	442.2	1782.0
26	0.5430	447.9	1805.0
27	0.5529	437.1	1768.0
28	0.5535	443.6	1795.0
29	0.5642	437.7	1780.0
30	0.5747	431.2	1764.0
31	0.5853	424.3	1748.0
32	0.5963	416.7	1731.0
33	0.6077	409.3	1717.0
34	0.6194	401.2	1702.0
35	0.6316	393.2	1690.0
36	0.6464	381.9	1671.0
37	0.6615	369.9	1652.0
38	0.6764	357.4	1633.0
39	0.6907	344.8	1614.0
40	0.7106	326.0	1585.0
41	0.7288	310.5	1571.0
42	0.7450	293.3	1544.0
43	0.7638	274.6	1522.0
44	0.7881	248.7	1489.0
45	0.8093	225.3	1460.0
46	0.8306	200.8	1427.0
47	0.8553	173.5	1402.0
48	0.8796	145.4	1373.0
49	0.9042	114.1	1317.0
50	0.9347	75.4	1236.0
51	0.9615	42.2	1140.0

TABLE A15:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-BUTANOL+N-HEPTANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0305	493.0	16674.0
2	0.0617	702.6	12136.0
3	0.1159	885.0	8637.0
4	0.1648	980.3	7122.0
5	0.2091	1038.2	6278.0
6	0.2490	1073.6	5741.0
7	0.2860	1094.3	5359.0
8	0.3192	1104.8	5084.0
9	0.3492	1107.2	4872.0
10	0.3770	1103.9	4700.0
11	0.4026	1095.5	4555.0
12	0.4252	1087.1	4448.0
13	0.4465	1074.6	4348.0
14	0.4657	1061.0	4264.0
15	0.4847	1046.0	4188.0
16	0.5024	1030.2	4121.0
17	0.5189	1013.8	4061.0
18	0.5345	996.7	4006.0
19	0.5491	979.7	3957.0
20	0.5625	963.0	3913.0
21	0.5749	946.5	3873.0
22	0.5863	930.7	3837.0
23	0.5979	904.7	3763.0
24	0.5996	911.3	3796.0
25	0.6076	890.5	3735.0
26	0.6090	897.2	3768.0
27	0.6173	875.0	3704.0
28	0.6180	883.6	3743.0
29	0.6272	859.1	3674.0
30	0.6280	867.9	3715.0
31	0.6373	841.2	3639.0
32	0.6476	826.6	3622.0
33	0.6585	808.0	3593.0
34	0.6697	787.7	3561.0
35	0.6813	767.3	3534.0
36	0.6933	744.2	3500.0
37	0.7057	720.5	3469.0
38	0.7186	694.2	3433.0
39	0.7321	666.6	3399.0
40	0.7462	636.9	3363.0
41	0.7637	601.1	3331.0
42	0.7790	567.4	3296.0
43	0.7949	532.0	3263.0
44	0.8114	493.4	3224.0
45	0.8288	450.8	3177.0
46	0.8463	408.0	3137.0
47	0.8657	363.8	3129.0
48	0.8856	312.8	3087.0
49	0.9065	257.5	3038.0
50	0.9284	199.4	3000.0
51	0.9514	136.6	2955.0
52	0.9752	70.8	2928.0

TABLE A16:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-BUTANOL+N-OCTANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0338	539.8	16529.0
2	0.0708	778.6	11835.0
3	0.1301	970.4	8574.0
4	0.1820	1066.1	7161.0
5	0.2288	1123.1	6365.0
6	0.2705	1157.1	5864.0
7	0.3074	1175.7	5522.0
8	0.3417	1183.2	5260.0
9	0.3721	1183.9	5067.0
10	0.4001	1178.3	4909.0
11	0.4254	1170.4	4788.0
12	0.4488	1158.0	4681.0
13	0.4699	1144.1	4593.0
14	0.4896	1128.5	4516.0
15	0.5072	1113.0	4453.0
16	0.5234	1097.1	4398.0
17	0.5393	1080.5	4349.0
18	0.5550	1061.5	4298.0
19	0.5691	1043.9	4257.0
20	0.5822	1026.5	4220.0
21	0.5945	1008.9	4185.0
22	0.6087	987.0	4144.0
23	0.6178	973.5	4123.0
24	0.6230	949.1	4041.0
25	0.6280	957.1	4097.0
26	0.6324	933.8	4017.0
27	0.6381	940.3	4072.0
28	0.6420	917.0	3990.0
29	0.6473	924.6	4050.0
30	0.6519	900.2	3967.0
31	0.6565	908.6	4029.0
32	0.6620	882.0	3942.0
33	0.6724	862.2	3914.0
34	0.6836	840.7	3887.0
35	0.6948	818.5	3860.0
36	0.7067	794.7	3834.0
37	0.7187	769.3	3805.0
38	0.7308	743.3	3778.0
39	0.7435	715.2	3750.0
40	0.7567	685.6	3724.0
41	0.7705	653.0	3693.0
42	0.7839	621.2	3667.0
43	0.7984	585.7	3639.0
44	0.8133	547.2	3604.0
45	0.8291	506.8	3577.0
46	0.8452	464.2	3548.0
47	0.8620	418.1	3515.0
48	0.8796	369.4	3488.0
49	0.8978	316.8	3453.0
50	0.9169	260.4	3417.0
51	0.9369	200.0	3383.0
52	0.9568	138.6	3353.0
53	0.9786	69.2	3304.0

TABLE A17:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-BUTANOL+N-NONANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0361	578.9	16637.0
2	0.0719	821.5	12311.0
3	0.1347	1031.4	8849.0
4	0.1900	1137.2	7389.0
5	0.2391	1197.5	6582.0
6	0.2829	1231.8	6072.0
7	0.3219	1249.4	5724.0
8	0.3575	1256.0	5468.0
9	0.3900	1254.0	5271.0
10	0.4189	1246.3	5120.0
11	0.4456	1234.5	4997.0
12	0.4697	1219.5	4896.0
13	0.4908	1203.1	4814.0
14	0.5108	1185.2	4743.0
15	0.5286	1167.7	4686.0
16	0.5453	1149.0	4634.0
17	0.5590	1132.0	4592.0
18	0.5731	1114.2	4554.0
19	0.5871	1095.0	4517.0
20	0.6005	1075.7	4484.0
21	0.6130	1056.2	4452.0
22	0.6248	1036.4	4421.0
23	0.6353	1018.5	4396.0
24	0.6448	1002.5	4377.0
25	0.6477	997.2	4370.0
26	0.6542	985.4	4356.0
27	0.6566	980.8	4350.0
28	0.6633	968.4	4336.0
29	0.6658	963.0	4328.0
30	0.6723	951.3	4318.0
31	0.6753	944.6	4308.0
32	0.6849	925.6	4289.0
33	0.6949	905.5	4271.0
34	0.7051	882.5	4244.0
35	0.7159	859.5	4226.0
36	0.7268	835.2	4206.0
37	0.7381	809.0	4185.0
38	0.7497	781.6	4165.0
39	0.7616	752.2	4143.0
40	0.7739	721.3	4122.0
41	0.7864	688.5	4099.0
42	0.7995	653.2	4075.0
43	0.8131	615.3	4049.0
44	0.8272	575.8	4028.0
45	0.8420	532.9	4006.0
46	0.8572	487.8	3985.0
47	0.8730	438.8	3958.0
48	0.8895	386.6	3933.0
49	0.9062	333.0	3918.0
50	0.9236	273.9	3881.0
51	0.9415	212.8	3864.0
52	0.9603	146.0	3830.0
53	0.9798	75.5	3815.0

TABLE A18:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-BUTANOL+N-DODECANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0447	717.5	16802.0
2	0.0896	1007.6	12352.0
3	0.1668	1247.7	8978.0
4	0.2322	1358.5	7620.0
5	0.2878	1413.3	6895.0
6	0.3361	1435.7	6434.0
7	0.3786	1443.8	6137.0
8	0.4160	1438.7	5922.0
9	0.4494	1426.5	5765.0
10	0.4796	1407.9	5641.0
11	0.5064	1386.0	5545.0
12	0.5307	1362.3	5470.0
13	0.5523	1338.2	5412.0
14	0.5720	1313.4	5365.0
15	0.5905	1286.7	5321.0
16	0.6073	1261.1	5288.0
17	0.6229	1235.1	5258.0
18	0.6375	1209.3	5233.0
19	0.6510	1183.5	5209.0
20	0.6629	1160.7	5194.0
21	0.6739	1138.6	5181.0
22	0.6847	1115.7	5168.0
23	0.6948	1093.3	5156.0
24	0.6975	1086.8	5151.0
25	0.7040	1072.6	5147.0
26	0.7058	1067.9	5143.0
27	0.7125	1052.5	5138.0
28	0.7142	1047.3	5131.0
29	0.7202	1034.0	5131.0
30	0.7228	1026.8	5125.0
31	0.7316	1004.4	5115.0
32	0.7406	980.9	5106.0
33	0.7595	930.3	5093.0
34	0.7694	902.7	5088.0
35	0.7793	872.5	5073.0
36	0.7895	843.9	5078.0
37	0.8002	811.6	5076.0
38	0.8111	776.7	5069.0
39	0.8221	742.1	5074.0
40	0.8338	703.3	5075.0
41	0.8459	661.5	5075.0
42	0.8582	618.4	5082.0
43	0.8708	571.8	5082.0
44	0.8837	522.7	5086.0
45	0.8966	472.3	5095.0
46	0.9100	417.9	5103.0
47	0.9242	358.3	5114.0
48	0.9387	295.5	5135.0
49	0.9534	228.9	5151.0
50	0.9683	158.3	5156.0
51	0.9841	80.5	5144.0

TABLE A19:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-PENTANOL+N-OCTANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0277	464.7	17254.0
2	0.0567	684.8	12804.0
3	0.1087	877.1	9053.0
4	0.1560	974.4	7401.0
5	0.1994	1032.2	6466.0
6	0.2377	1067.4	5891.0
7	0.2729	1089.6	5491.0
8	0.3054	1101.0	5190.0
9	0.3350	1105.9	4964.0
10	0.3623	1106.2	4788.0
11	0.3874	1102.1	4644.0
12	0.4105	1095.2	4526.0
13	0.4315	1086.7	4430.0
14	0.4510	1075.8	4345.0
15	0.4688	1064.6	4275.0
16	0.4863	1052.0	4211.0
17	0.5024	1038.5	4154.0
18	0.5170	1025.1	4105.0
19	0.5304	1011.2	4060.0
20	0.5427	998.2	4022.0
21	0.5552	984.4	3986.0
22	0.5673	970.1	3952.0
23	0.5732	951.9	3891.0
24	0.5810	951.4	3908.0
25	0.5826	939.4	3863.0
26	0.5910	938.4	3882.0
27	0.5927	925.8	3835.0
28	0.6012	924.0	3854.0
29	0.6032	910.7	3805.0
30	0.6106	910.6	3830.0
31	0.6139	894.8	3775.0
32	0.6198	896.9	3806.0
33	0.6248	878.9	3749.0
34	0.6286	883.4	3784.0
35	0.6364	860.6	3719.0
36	0.6483	840.9	3688.0
37	0.6605	820.3	3658.0
38	0.6734	797.0	3624.0
39	0.6867	773.0	3593.0
40	0.7005	746.9	3560.0
41	0.7150	718.1	3524.0
42	0.7299	688.6	3493.0
43	0.7453	655.7	3454.0
44	0.7617	621.0	3421.0
45	0.7784	583.4	3382.0
46	0.7960	541.9	3337.0
47	0.8146	499.3	3306.0
48	0.8344	450.6	3261.0
49	0.8549	398.9	3216.0
50	0.8766	343.2	3173.0
51	0.8988	283.7	3119.0
52	0.9228	219.1	3076.0
53	0.9473	150.7	3018.0
54	0.9737	76.1	2970.0

TABLE A20:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-PENTANOL+N-NONANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0302	506.2	17293.0
2	0.0611	738.1	12867.0
3	0.1167	944.1	9159.0
4	0.1658	1044.9	7555.0
5	0.2104	1104.6	6649.0
6	0.2510	1141.7	6073.0
7	0.2875	1162.3	5674.0
8	0.3207	1174.0	5389.0
9	0.3509	1177.6	5170.0
10	0.3778	1220.0	5190.0
11	0.4029	1209.1	5026.0
12	0.4259	1228.4	5024.0
13	0.4473	1211.9	4902.0
14	0.4666	1194.6	4800.0
15	0.4845	1176.9	4712.0
16	0.5014	1158.5	4634.0
17	0.5173	1140.1	4566.0
18	0.5322	1122.6	4509.0
19	0.5462	1105.0	4458.0
20	0.5601	1086.1	4408.0
21	0.5730	1067.5	4363.0
22	0.5855	1048.7	4321.0
23	0.5964	1031.9	4287.0
24	0.6069	1015.1	4255.0
25	0.6109	993.6	4180.0
26	0.6168	998.6	4225.0
27	0.6205	978.2	4154.0
28	0.6250	985.1	4203.0
29	0.6303	962.6	4131.0
30	0.6337	970.0	4179.0
31	0.6401	945.9	4106.0
32	0.6503	927.8	4080.0
33	0.6612	908.6	4056.0
34	0.6719	889.3	4034.0
35	0.6830	866.7	4003.0
36	0.6949	844.0	3981.0
37	0.7068	819.6	3955.0
38	0.7187	794.1	3928.0
39	0.7317	766.0	3902.0
40	0.7451	736.2	3876.0
41	0.7589	703.9	3847.0
42	0.7732	668.8	3814.0
43	0.7882	632.2	3787.0
44	0.8037	592.3	3754.0
45	0.8194	551.7	3728.0
46	0.8363	505.7	3694.0
47	0.8539	457.2	3665.0
48	0.8722	404.1	3625.0
49	0.8911	348.2	3588.0
50	0.9109	287.7	3545.0
51	0.9316	222.3	3489.0
52	0.9532	153.5	3441.0
53	0.9760	79.0	3374.0

TABLE A21:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-PENTANOL+N-DODECANE
DELTA H IN JOULES/MOLE

N	X. ALC	DELTA H	DEL H/X1X2
1	0.0399	641.9	16756.0
2	0.0762	908.2	12902.0
3	0.1440	1149.2	9323.0
4	0.2032	1260.8	7787.0
5	0.2560	1321.6	6939.0
6	0.3014	1353.5	6428.0
7	0.3419	1367.4	6077.0
8	0.3772	1371.0	5836.0
9	0.4101	1365.4	5644.0
10	0.4398	1355.3	5501.0
11	0.4657	1343.9	5401.0
12	0.4893	1327.9	5314.0
13	0.5100	1311.0	5246.0
14	0.5276	1295.8	5199.0
15	0.5454	1277.4	5152.0
16	0.5614	1260.5	5119.0
17	0.5774	1240.9	5085.0
18	0.5924	1220.4	5054.0
19	0.6071	1199.1	5027.0
20	0.6197	1148.7	4874.0
21	0.6316	1131.8	4864.0
22	0.6434	1143.1	4982.0
23	0.6544	1123.8	4969.0
24	0.6641	1090.6	4889.0
25	0.6648	1104.4	4956.0
26	0.6730	1072.6	4874.0
27	0.6743	1086.2	4946.0
28	0.6817	1055.6	4865.0
29	0.6833	1068.4	4937.0
30	0.6907	1035.9	4849.0
31	0.6918	1050.9	4929.0
32	0.6983	1037.0	4922.0
33	0.7000	1016.4	4840.0
34	0.7096	994.9	4828.0
35	0.7193	972.0	4814.0
36	0.7298	947.1	4803.0
37	0.7404	921.3	4793.0
38	0.7510	894.4	4783.0
39	0.7618	865.6	4770.0
40	0.7732	833.5	4753.0
41	0.7852	800.5	4746.0
42	0.7972	765.7	4736.0
43	0.8098	728.4	4729.0
44	0.8227	687.8	4715.0
45	0.8358	646.4	4710.0
46	0.8495	601.0	4701.0
47	0.8641	550.6	4689.0
48	0.8791	497.8	4684.0
49	0.8944	441.6	4676.0
50	0.9102	380.4	4654.0
51	0.9270	314.9	4653.0
52	0.9445	243.3	4642.0
53	0.9627	166.6	4640.0
54	0.9811	85.1	4587.0

TABLE A22:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-HEXANOL+N-OCTANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0243	410.7	17321.0
2	0.0491	620.8	13296.0
3	0.0954	807.1	9352.0
4	0.1379	899.7	7568.0
5	0.1773	955.7	6552.0
6	0.2127	988.6	5914.0
7	0.2435	1008.9	5477.0
8	0.2732	1022.0	5147.0
9	0.3010	1028.6	4889.0
10	0.3268	1030.5	4684.0
11	0.3499	1029.5	4526.0
12	0.3719	1025.9	4392.0
13	0.3933	1019.8	4274.0
14	0.4127	1012.4	4177.0
15	0.4310	1003.5	4092.0
16	0.4478	994.3	4021.0
17	0.4634	984.2	3958.0
18	0.4781	974.4	3905.0
19	0.4931	962.1	3849.0
20	0.5061	950.9	3804.0
21	0.5181	939.8	3764.0
22	0.5287	930.2	3733.0
23	0.5401	919.3	3701.0
24	0.5474	899.8	3632.0
25	0.5514	906.8	3666.0
26	0.5570	889.8	3606.0
27	0.5617	895.2	3636.0
28	0.5670	878.4	3578.0
29	0.5718	883.2	3607.0
30	0.5775	865.9	3549.0
31	0.5809	872.1	3582.0
32	0.5883	852.3	3519.0
33	0.5997	836.8	3486.0
34	0.6114	820.9	3455.0
35	0.6237	803.4	3423.0
36	0.6366	784.2	3390.0
37	0.6501	763.4	3356.0
38	0.6640	742.3	3327.0
39	0.6783	718.3	3292.0
40	0.6932	692.7	3257.0
41	0.7086	664.9	3220.0
42	0.7249	635.2	3185.0
43	0.7416	603.1	3147.0
44	0.7592	568.6	3110.0
45	0.7786	527.8	3062.0
46	0.7986	485.6	3019.0
47	0.8196	439.9	2975.0
48	0.8411	392.1	2934.0
49	0.8638	339.5	2886.0
50	0.8887	280.5	2836.0
51	0.9143	217.6	2777.0
52	0.9413	150.3	2721.0
53	0.9696	77.9	2644.0

TABLE A23:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-OCTANOL+N-HEPTANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0170	289.7	17334.0
2	0.0336	417.0	12841.0
3	0.0657	635.3	10350.0
4	0.0971	720.7	8221.0
5	0.1276	774.6	6958.0
6	0.1562	808.2	6132.0
7	0.1825	829.1	5557.0
8	0.2079	842.3	5115.0
9	0.2302	851.7	4806.0
10	0.2514	855.4	4545.0
11	0.2701	858.6	4355.0
12	0.2897	858.9	4174.0
13	0.3078	859.2	4028.0
14	0.3263	855.8	3893.0
15	0.3433	851.5	3777.0
16	0.3591	847.2	3681.0
17	0.3735	842.2	3599.0
18	0.3875	836.4	3524.0
19	0.4001	830.7	3461.0
20	0.4120	825.1	3406.0
21	0.4237	819.5	3356.0
22	0.4354	813.2	3308.0
23	0.4472	806.4	3262.0
24	0.4580	800.1	3223.0
25	0.4613	791.7	3186.0
26	0.4695	792.5	3182.0
27	0.4712	784.1	3147.0
28	0.4817	777.7	3115.0
29	0.4819	782.7	3135.0
30	0.4918	776.0	3105.0
31	0.4922	768.1	3073.0
32	0.5016	768.2	3073.0
33	0.5036	757.5	3030.0
34	0.5103	760.7	3044.0
35	0.5153	747.0	2991.0
36	0.5178	754.3	3021.0
37	0.5256	747.8	2999.0
38	0.5275	735.8	2952.0
39	0.5402	723.3	2912.0
40	0.5535	709.8	2872.0
41	0.5675	695.3	2833.0
42	0.5821	678.7	2790.0
43	0.5975	661.4	2750.0
44	0.6137	642.0	2708.0
45	0.6308	619.5	2660.0
46	0.6488	596.8	2619.0
47	0.6680	571.7	2578.0
48	0.6885	542.8	2531.0
49	0.7111	509.7	2481.0
50	0.7348	474.1	2433.0
51	0.7598	434.4	2380.0
52	0.7868	389.8	2324.0
53	0.8146	343.6	2275.0
54	0.8462	287.2	2207.0
55	0.8797	226.8	2143.0
56	0.9165	157.5	2058.0
57	0.9573	81.1	1985.0

TABLE A24:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-OCTANOL+N-OCTANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0189	330.5	17823.0
2	0.0348	494.9	14734.0
3	0.0693	676.8	10493.0
4	0.1020	771.1	8418.0
5	0.1324	827.4	7203.0
6	0.1607	863.3	6401.0
7	0.1887	888.5	5804.0
8	0.2149	903.8	5357.0
9	0.2384	914.9	5039.0
10	0.2580	918.9	4800.0
11	0.2750	922.7	4628.0
12	0.2920	924.1	4470.0
13	0.3104	923.4	4314.0
14	0.3279	921.9	4183.0
15	0.3456	918.4	4061.0
16	0.3613	914.7	3964.0
17	0.3766	910.4	3878.0
18	0.3918	904.6	3796.0
19	0.4059	898.3	3725.0
20	0.4192	891.6	3662.0
21	0.4323	884.5	3604.0
22	0.4453	876.4	3548.0
23	0.4568	868.2	3499.0
24	0.4679	860.2	3455.0
25	0.4785	852.4	3416.0
26	0.4838	845.6	3386.0
27	0.4878	846.2	3387.0
28	0.4935	838.6	3355.0
29	0.4984	838.2	3353.0
30	0.5034	830.0	3320.0
31	0.5084	830.5	3323.0
32	0.5141	821.1	3287.0
33	0.5183	822.4	3294.0
34	0.5253	810.4	3250.0
35	0.5293	811.7	3258.0
36	0.5367	798.9	3213.0
37	0.5489	786.9	3178.0
38	0.5614	773.9	3143.0
39	0.5747	759.2	3106.0
40	0.5884	743.0	3068.0
41	0.6031	725.5	3031.0
42	0.6183	705.9	2991.0
43	0.6346	684.3	2951.0
44	0.6517	660.5	2910.0
45	0.6696	634.7	2869.0
46	0.6884	606.6	2828.0
47	0.7088	575.2	2787.0
48	0.7311	539.5	2744.0
49	0.7780	457.2	2647.0
50	0.8035	409.9	2596.0
51	0.8306	358.5	2548.0
52	0.8596	300.8	2492.0
53	0.8909	237.2	2440.0
54	0.9249	165.8	2387.0
55	0.9608	87.1	2312.0

TABLE A25:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-OCTANOL+N-NONANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0223	334.5	15340.0
2	0.0431	542.6	13157.0
3	0.0844	744.8	9638.0
4	0.1223	839.5	7921.0
5	0.1580	895.9	6734.0
6	0.1904	930.6	6037.0
7	0.2213	953.3	5532.0
8	0.2496	967.8	5167.0
9	0.2743	974.6	4896.0
10	0.2959	976.7	4688.0
11	0.3175	977.9	4513.0
12	0.3384	977.9	4368.0
13	0.3582	976.8	4249.0
14	0.3770	972.1	4139.0
15	0.3949	966.3	4044.0
16	0.4113	960.3	3966.0
17	0.4268	953.1	3896.0
18	0.4296	965.2	3939.0
19	0.4434	957.3	3879.0
20	0.4573	920.2	3708.0
21	0.4705	939.7	3772.0
22	0.4828	930.6	3727.0
23	0.4947	921.1	3685.0
24	0.5058	912.4	3650.0
25	0.5115	900.3	3603.0
26	0.5165	904.0	3620.0
27	0.5213	890.4	3568.0
28	0.5276	894.5	3589.0
29	0.5315	880.0	3534.0
30	0.5376	885.7	3563.0
31	0.5420	870.1	3505.0
32	0.5476	876.0	3536.0
33	0.5529	858.3	3472.0
34	0.5577	865.1	3507.0
35	0.5646	844.9	3437.0
36	0.5658	856.4	3486.0
37	0.5763	831.2	3404.0
38	0.5886	816.3	3371.0
39	0.6021	798.7	3334.0
40	0.6154	780.1	3296.0
41	0.6292	761.5	3264.0
42	0.6444	739.9	3229.0
43	0.6606	715.7	3192.0
44	0.6770	690.1	3156.0
45	0.6942	667.3	3120.0
46	0.7129	630.4	3080.0
47	0.7321	596.6	3042.0
48	0.7521	559.3	3000.0
49	0.7731	519.1	2959.0
50	0.7954	474.1	2913.0
51	0.8198	423.8	2869.0
52	0.8452	369.4	2823.0
53	0.8727	307.7	2770.0
54	0.9017	240.0	2708.0
55	0.9330	166.2	2658.0
56	0.9653	87.2	2604.0

TABLE A26:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-OCTANOL+N-DODECANE
DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0271	473.1	17943.0
2	0.0547	732.9	14174.0
3	0.1037	952.7	10250.0
4	0.1481	1057.7	8393.0
5	0.1885	1117.0	7302.0
6	0.2258	1149.8	6577.0
7	0.2597	1167.0	6070.0
8	0.2912	1176.5	5700.0
9	0.3190	1177.4	5420.0
10	0.3449	1175.6	5203.0
11	0.3698	1169.0	5016.0
12	0.3928	1160.3	4865.0
13	0.4142	1150.8	4743.0
14	0.4341	1140.1	4641.0
15	0.4523	1129.1	4558.0
16	0.4699	1116.2	4481.0
17	0.4865	1101.7	4410.0
18	0.5013	1087.2	4349.0
19	0.5149	1073.8	4299.0
20	0.5279	1060.9	4257.0
21	0.5402	1048.7	4222.0
22	0.5523	1035.8	4189.0
23	0.5645	1021.5	4155.0
24	0.5760	1001.1	4099.0
25	0.5761	1007.1	4124.0
26	0.5851	989.5	4076.0
27	0.5864	993.9	4098.0
28	0.5947	976.7	4052.0
29	0.5967	979.4	4070.0
30	0.6047	962.8	4028.0
31	0.6058	966.7	4048.0
32	0.6145	954.4	4029.0
33	0.6156	947.7	4005.0
34	0.6265	930.8	3978.0
35	0.6379	912.6	3951.0
36	0.6498	894.1	3929.0
37	0.6620	873.1	3902.0
38	0.6748	851.7	3881.0
39	0.6879	827.9	3956.0
40	0.7014	802.1	3830.0
41	0.7150	775.2	3804.0
42	0.7298	745.8	3782.0
43	0.7449	713.9	3757.0
44	0.7615	677.3	3729.0
45	0.7793	637.6	3707.0
46	0.7973	594.6	3679.0
47	0.8157	548.6	3649.0
48	0.8353	499.0	3627.0
49	0.8552	445.7	3599.0
50	0.8772	383.3	3558.0
51	0.8994	319.9	3536.0
52	0.9227	249.1	3493.0
53	0.9470	174.8	3482.0
54	0.9724	91.1	3393.0

TABLE A27:

HEATS OF MIXING OF SYSTEM N-[illegible]TANOL - N-HEXANE
TEMP=25 DEG C. DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0205	229.8	11442.2
2	0.0459	311.3	7114.2
3	0.0880	385.4	4802.8
4	0.1277	431.8	3875.1
5	0.1637	462.5	3377.7
6	0.1962	484.8	3074.3
7	0.2269	501.8	2960.3
8	0.2558	512.8	2699.0
9	0.2815	521.4	2577.8
10	0.3058	525.9	2477.5
11	0.3291	529.0	2395.8
12	0.3506	529.1	2323.6
13	0.3707	527.5	2261.1
14	0.3896	524.5	2205.6
15	0.4072	519.7	2153.1
16	0.4243	515.4	2110.0
17	0.4404	509.5	2067.2
18	0.4554	503.2	2028.8
19	0.4700	496.5	1993.0
20	0.4835	489.4	1959.8
21	0.4962	482.1	1928.5
22	0.5107	473.5	1894.9
23	0.5224	465.6	1866.1
24	0.5318	458.8	1842.6
25	0.5325	458.3	1841.1
26	0.5410	452.2	1821.1
27	0.5423	451.6	1819.6
28	0.5504	445.7	1801.0
29	0.5527	443.3	1792.9
30	0.5595	439.0	1781.1
31	0.5632	435.6	1770.5
32	0.5746	426.3	1743.8
33	0.5858	417.0	1718.5
34	0.5980	406.7	1691.8
35	0.6108	396.1	1666.1
36	0.6238	384.1	1636.8
37	0.6371	372.0	1609.1
38	0.6509	359.1	1580.5
39	0.6652	345.8	1553.0
40	0.6805	331.0	1522.5
41	0.6964	315.2	1490.9
42	0.7131	298.7	1459.9
43	0.7308	280.7	1426.6
44	0.7493	262.0	1394.9
45	0.7688	241.8	1360.1
46	0.7897	219.7	1322.9
47	0.8107	198.3	1291.7
48	0.8335	173.5	1250.5
49	0.8576	148.6	1217.0
50	0.8825	122.5	1182.1
51	0.9104	93.0	1140.4
52	0.9375	65.4	1115.2
53	0.9688	32.4	1074.7

TABLE A28:

HEATS OF MIXING OF SYSTEM N-PENTANOL - 2,2-DIMETHYLBUTANE
TEMP=25 DEG C. DELTA H IN JOULES/MOLE

N	X-ALC	DELTA H	DEL H/X1X2
1	0.0196	221.4	11524.3
2	0.0458	304.9	6982.7
3	0.0887	376.5	4659.3
4	0.1280	418.8	3752.8
5	0.1644	448.0	3260.8
6	0.1975	469.2	2960.2
7	0.2277	483.9	2752.0
8	0.2559	494.4	2596.3
9	0.2820	501.3	2475.9
10	0.3065	505.5	2378.3
11	0.3298	507.5	2296.2
12	0.3516	507.0	2223.7
13	0.3726	504.9	2159.7
14	0.3919	501.0	2102.0
15	0.4110	495.8	2048.2
16	0.4281	490.3	2002.8
17	0.4442	483.4	1957.9
18	0.4597	476.8	1919.7
19	0.4738	469.3	1882.5
20	0.4876	462.3	1850.2
21	0.5000	454.3	1817.0
22	0.5123	447.1	1789.5
23	0.5233	439.1	1760.4
24	0.5318	436.8	1754.3
25	0.5367	430.7	1732.2
26	0.5472	423.0	1707.0
27	0.5418	429.7	1730.7
28	0.5518	422.5	1708.1
29	0.5574	415.6	1684.6
30	0.5622	413.9	1681.6
31	0.5732	405.6	1658.1
32	0.5844	397.0	1634.6
33	0.5961	387.1	1607.9
34	0.6085	376.3	1579.4
35	0.6217	365.0	1551.7
36	0.6353	352.6	1522.0
37	0.6491	340.4	1494.3
38	0.6637	326.8	1464.2
39	0.6794	311.8	1431.3
40	0.6954	296.9	1401.7
41	0.7119	281.0	1370.0
42	0.7294	264.3	1339.2
43	0.7477	246.2	1305.2
44	0.7672	227.0	1271.3
45	0.7878	207.0	1238.1
46	0.8092	186.3	1206.5
47	0.8320	163.9	1172.7
48	0.8558	140.2	1135.8
49	0.8814	114.6	1096.2
50	0.9081	88.8	1064.3
51	0.9365	60.9	1024.6
52	0.9672	31.4	990.2

TABLE A29:

HEATS OF MIXING OF SYSTEM N-PENTANOL - 2,3-DIMETHYLBUTANE
TEMP=25 DEG.C. DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0217	233.6	10992.9
2	0.0452	305.5	7080.3
3	0.0877	377.5	4718.5
4	0.1270	420.4	3791.6
5	0.1627	449.9	3303.4
6	0.1959	471.5	2994.0
7	0.2268	486.4	2773.8
8	0.2553	497.6	2616.7
9	0.2818	505.0	2495.2
10	0.3070	509.0	2392.3
11	0.3341	508.8	2287.1
12	0.3551	509.3	2224.1
13	0.3757	506.7	2160.1
14	0.3942	502.5	2104.2
15	0.4114	497.9	2056.2
16	0.4279	492.4	2011.3
17	0.4435	486.1	1969.8
18	0.4581	479.8	1932.7
19	0.4723	472.2	1894.7
20	0.4855	465.2	1862.4
21	0.4984	457.7	1830.7
22	0.5110	449.9	1800.4
23	0.5231	441.9	1771.2
24	0.5327	434.8	1746.8
25	0.5342	432.7	1738.9
26	0.5423	428.0	1724.3
27	0.5439	425.7	1716.0
28	0.5515	421.4	1703.8
29	0.5540	417.9	1691.2
30	0.5647	409.7	1666.9
31	0.5759	400.8	1640.9
32	0.5870	391.6	1615.3
33	0.5988	381.5	1588.2
34	0.6108	371.3	1561.9
35	0.6238	359.9	1533.5
36	0.6371	348.0	1505.0
37	0.6511	335.7	1477.8
38	0.6656	321.9	1446.1
39	0.6807	307.3	1413.8
40	0.6958	293.4	1386.2
41	0.7122	277.6	1354.2
42	0.7296	260.8	1322.3
43	0.7478	243.2	1289.4
44	0.7681	222.7	1250.3
45	0.7880	203.1	1215.9
46	0.8089	183.0	1183.7
47	0.8313	160.7	1146.1
48	0.8552	137.4	1109.5
49	0.8807	112.6	1072.0
50	0.9077	86.6	1033.1
51	0.9373	58.5	995.2
52	0.9669	30.1	939.4

TABLE A30:

HEATS OF MIXING OF SYSTEM N-PENTANOL - 2-METHYLPENTANE
TEMP=25 DEG C. DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0194	213.6	11216.1
2	0.0446	295.2	6922.2
3	0.0862	368.1	4673.6
4	0.1248	413.3	3783.9
5	0.1612	444.0	3283.3
6	0.1941	466.5	2982.4
7	0.2247	483.1	2772.4
8	0.2532	494.8	2616.4
9	0.2795	502.4	2495.1
10	0.3040	508.0	2400.8
11	0.3273	510.4	2318.3
12	0.3487	510.6	2248.1
13	0.3684	509.3	2188.7
14	0.3878	506.7	2134.3
15	0.4063	502.3	2082.1
16	0.4237	497.4	2037.1
17	0.4397	491.8	1996.3
18	0.4552	485.7	1958.5
19	0.4701	478.6	1921.5
20	0.4841	471.3	1887.0
21	0.4975	463.5	1853.9
22	0.5096	456.3	1825.7
23	0.5207	449.3	1800.4
24	0.5314	442.2	1776.0
25	0.5324	447.4	1797.1
26	0.5421	435.0	1752.3
27	0.5422	440.6	1774.8
28	0.5516	428.0	1730.6
29	0.5524	433.0	1751.0
30	0.5630	424.7	1726.2
31	0.5739	416.0	1701.2
32	0.5855	406.6	1675.5
33	0.5974	396.2	1647.4
34	0.6098	386.3	1623.5
35	0.6230	374.6	1595.1
36	0.6363	362.2	1564.9
37	0.6504	349.5	1536.9
38	0.6650	335.9	1507.7
39	0.6803	321.2	1476.7
40	0.6961	306.0	1446.3
41	0.7129	289.4	1413.9
42	0.7301	272.3	1381.8
43	0.7486	253.6	1347.6
44	0.7675	234.7	1315.3
45	0.7873	214.7	1282.3
46	0.8087	193.4	1249.8
47	0.8315	169.6	1210.3
48	0.8563	145.6	1183.4
49	0.8815	119.5	1143.1
50	0.9078	92.8	1108.9
51	0.9366	64.3	1081.8
52	0.9668	33.4	1040.2

TABLE A31:

HEATS OF MIXING OF SYSTEM N-PENTANOL - 3-METHYLPENTANE
TEMP=25 DEG C. DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0206	226.6	11230.4
2	0.0446	303.7	7132.5
3	0.0860	375.9	4784.5
4	0.1257	421.2	3833.6
5	0.1618	452.1	3333.9
6	0.1944	474.3	3029.2
7	0.2251	489.9	2808.4
8	0.2538	501.3	2647.3
9	0.2808	509.9	2525.1
10	0.3061	514.1	2420.4
11	0.3293	516.6	2338.9
12	0.3513	515.9	2263.9
13	0.3709	514.5	2205.2
14	0.3934	509.4	2134.5
15	0.4105	505.8	2090.4
16	0.4274	500.5	2045.2
17	0.4431	494.3	2003.2
18	0.4576	487.9	1965.6
19	0.4711	480.8	1929.8
20	0.4842	473.8	1897.2
21	0.4965	466.7	1867.0
22	0.5090	459.3	1837.8
23	0.5160	457.9	1833.4
24	0.5204	451.6	1809.3
25	0.5259	451.2	1809.6
26	0.5315	444.4	1784.5
27	0.5361	443.7	1783.9
28	0.5422	436.6	1758.9
29	0.5468	434.8	1754.6
30	0.5515	429.5	1736.4
31	0.5576	426.1	1727.5
32	0.5688	417.6	1702.8
33	0.5808	407.2	1672.6
34	0.5933	396.4	1642.7
35	0.6064	384.9	1612.5
36	0.6198	372.5	1581.0
37	0.6340	359.9	1550.9
38	0.6490	345.1	1514.8
39	0.6646	331.0	1484.8
40	0.6812	315.2	1451.1
41	0.6982	299.0	1419.1
42	0.7163	281.1	1383.3
43	0.7353	262.5	1348.7
44	0.7549	242.4	1310.2
45	0.7760	221.3	1273.1
46	0.7984	199.1	1236.9
47	0.8222	175.1	1197.9
48	0.8467	150.4	1158.6
49	0.8728	124.4	1120.7
50	0.9022	95.3	1079.8
51	0.9333	64.7	1040.2
52	0.9651	32.9	978.3

TABLE A32:

HEATS OF MIXING OF SYSTEM ISOPENTANOL - N-HEXANE
TEMP=25 DEG C. DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0212	238.7	11481.3
2	0.0449	316.9	7390.6
3	0.0869	395.3	4981.3
4	0.1257	445.3	4050.9
5	0.1617	481.0	3548.8
6	0.1943	506.6	3236.9
7	0.2243	526.6	3026.1
8	0.2529	542.3	2869.9
9	0.2793	553.7	2750.9
10	0.3040	561.5	2653.7
11	0.3269	566.9	2576.4
12	0.3484	569.4	2508.1
13	0.3687	570.3	2450.2
14	0.3878	569.7	2399.5
15	0.4057	567.4	2353.2
16	0.4225	563.8	2310.6
17	0.4384	559.8	2273.6
18	0.4536	554.9	2238.8
19	0.4685	548.4	2202.3
20	0.4819	542.8	2173.9
21	0.4948	536.3	2145.5
22	0.5068	529.2	2117.3
23	0.5183	522.6	2093.4
24	0.5291	515.4	2068.8
25	0.5360	506.8	2037.7
26	0.5396	508.8	2048.0
27	0.5456	500.0	2016.8
28	0.5499	501.3	2025.3
29	0.5556	492.8	1995.9
30	0.5661	484.6	1972.8
31	0.5771	475.7	1949.0
32	0.5887	466.0	1924.4
33	0.6007	455.4	1898.6
34	0.6130	444.5	1873.6
35	0.6258	432.7	1847.6
36	0.6390	419.6	1819.0
37	0.6529	406.1	1792.0
38	0.6677	391.0	1762.4
39	0.6831	375.4	1734.4
40	0.6993	358.3	1703.6
41	0.7157	340.2	1671.7
42	0.7330	320.9	1639.8
43	0.7512	299.7	1603.7
44	0.7702	278.4	1572.5
45	0.7903	254.9	1538.0
46	0.8114	229.4	1499.3
47	0.8341	202.6	1464.5
48	0.8583	173.2	1423.9
49	0.8829	143.8	1390.9
50	0.9107	109.6	1347.8
51	0.9384	75.3	1302.0
52	0.9684	38.4	1255.2

TABLE A33:

HEATS OF MIXING OF SYSTEM ISOPENTANOL - 2,2-DIMETHYLBUTANE
TEMP=25 DEG C. DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0216	232.1	10980.7
2	0.0462	309.8	7028.2
3	0.0887	383.3	4740.9
4	0.1291	428.6	3812.4
5	0.1658	460.0	3325.4
6	0.1991	482.8	3028.4
7	0.2298	500.2	2825.9
8	0.2590	511.8	2666.7
9	0.2862	520.6	2548.3
10	0.3105	526.2	2457.8
11	0.3333	529.8	2384.2
12	0.3541	530.9	2321.0
13	0.3739	530.4	2265.6
14	0.3925	527.8	2213.4
15	0.4099	524.8	2169.6
16	0.4264	520.8	2129.4
17	0.4424	515.8	2090.8
18	0.4576	509.8	2053.9
19	0.4713	504.1	2023.3
20	0.4844	497.8	1993.0
21	0.4971	491.1	1964.4
22	0.5094	484.0	1936.6
23	0.5213	477.2	1912.2
24	0.5321	469.6	1886.3
25	0.5441	457.0	1842.5
26	0.5448	461.0	1858.9
27	0.5540	449.3	1818.3
28	0.5552	453.7	1837.3
29	0.5643	441.1	1794.1
30	0.5750	433.8	1775.3
31	0.5866	423.7	1747.3
32	0.5981	414.3	1723.6
33	0.6103	403.3	1695.8
34	0.6234	391.6	1668.0
35	0.6363	377.2	1629.9
36	0.6529	364.3	1607.4
37	0.6677	350.7	1580.7
38	0.6823	335.5	1547.5
39	0.6986	318.8	1514.1
40	0.7149	302.3	1483.4
41	0.7328	283.4	1447.5
42	0.7509	263.9	1411.2
43	0.7699	244.0	1377.3
44	0.7909	222.6	1346.0
45	0.8123	198.5	1302.0
46	0.8341	175.4	1267.7
47	0.8577	149.8	1227.7
48	0.8835	122.5	1190.6
49	0.9096	94.9	1154.4
50	0.9385	63.9	1107.1
51	0.9690	31.6	1052.3

TABLE A34:

HEATS OF MIXING OF SYSTEM ISOPENTANOL - 2,3-DIMETHYLBUTANE
TEMP=25 DEG C. DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0200	217.3	11081.6
2	0.0449	297.5	6941.6
3	0.0860	371.5	4724.5
4	0.1262	419.7	3804.6
5	0.1614	451.8	3338.1
6	0.1947	475.5	3033.0
7	0.2251	494.3	2834.1
8	0.2531	507.7	2685.3
9	0.2786	517.1	2572.8
10	0.3032	524.5	2482.7
11	0.3264	529.0	2406.3
12	0.3476	530.1	2337.4
13	0.3675	531.1	2284.9
14	0.3867	529.7	2233.7
15	0.4048	527.3	2188.7
16	0.4248	521.6	2134.7
17	0.4410	517.7	2100.1
18	0.4546	512.1	2065.3
19	0.4687	506.7	2034.8
20	0.4818	500.3	2003.9
21	0.4950	493.6	1974.7
22	0.5065	487.1	1948.9
23	0.5177	480.4	1924.0
24	0.5286	473.5	1900.3
25	0.5317	472.7	1898.3
26	0.5386	466.4	1876.9
27	0.5415	465.8	1876.0
28	0.5482	459.8	1856.4
29	0.5519	458.2	1852.9
30	0.5628	450.0	1828.6
31	0.5736	441.6	1805.4
32	0.5850	431.9	1779.0
33	0.5968	421.9	1753.3
34	0.6092	410.8	1725.7
35	0.6222	399.0	1697.5
36	0.6357	386.1	1667.2
37	0.6500	372.3	1636.5
38	0.6648	358.2	1607.3
39	0.6793	343.6	1577.0
40	0.6957	326.8	1543.8
41	0.7124	309.8	1512.4
42	0.7302	290.8	1476.2
43	0.7486	271.5	1443.0
44	0.7680	250.2	1404.5
45	0.7887	227.3	1364.2
46	0.8108	203.7	1328.3
47	0.8332	179.3	1290.7
48	0.8575	152.5	1247.8
49	0.8830	124.7	1206.3
50	0.9097	95.3	1159.3
51	0.9377	65.5	1121.0
52	0.9678	32.4	1039.2

TABLE A35:

HEATS OF MIXING OF SYSTEM ISOPENTANOL – 2-METHYLPENTANE
TEMP=25 DEG C. DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0217	241.9	11387.8
2	0.0462	319.4	7243.7
3	0.0886	395.7	4901.5
4	0.1281	442.2	3958.7
5	0.1649	475.4	3452.7
6	0.1984	498.7	3136.0
7	0.2291	517.1	2928.1
8	0.2578	531.1	2775.9
9	0.2839	540.2	2657.4
10	0.3091	547.0	2561.5
11	0.3317	550.0	2480.9
12	0.3533	551.6	2414.0
13	0.3730	551.8	2359.2
14	0.3918	549.8	2307.4
15	0.4098	547.1	2262.1
16	0.4265	543.1	2220.6
17	0.4423	538.0	2181.2
18	0.4576	532.7	2146.3
19	0.4718	526.0	2110.8
20	0.4847	519.6	2080.4
21	0.4977	513.1	2052.4
22	0.5102	506.1	2025.3
23	0.5220	498.5	1998.0
24	0.5331	491.1	1973.2
25	0.5361	486.9	1957.7
26	0.5439	484.0	1951.1
27	0.5459	479.8	1935.5
28	0.5543	476.4	1928.3
29	0.5560	471.9	1911.5
30	0.5666	463.5	1887.4
31	0.5779	454.8	1864.5
32	0.5894	444.4	1836.4
33	0.6012	435.1	1814.6
34	0.6136	424.3	1789.6
35	0.6267	412.3	1762.2
36	0.6401	399.1	1732.6
37	0.6540	385.3	1702.9
38	0.6688	370.9	1674.3
39	0.6847	355.3	1646.0
40	0.7010	338.2	1613.6
41	0.7177	320.3	1580.7
42	0.7355	301.3	1549.1
43	0.7540	281.1	1515.3
44	0.7731	259.7	1480.2
45	0.7931	237.2	1445.4
46	0.8143	213.4	1410.8
47	0.8366	187.7	1372.9
48	0.8608	159.5	1331.2
49	0.8855	131.5	1297.6
50	0.9109	101.7	1253.3
51	0.9390	69.6	1214.8
52	0.9688	36.0	1190.8

TABLE A36:

HEATS OF MIXING OF SYSTEM ISOPENTANOL - 3-METHYLPENTANE
TEMP=25 DEG C. DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0206	275.6	11196.9
2	0.0633	344.3	5803.5
3	0.1036	404.1	4349.7
4	0.1406	444.3	3677.6
5	0.1747	472.9	3279.5
6	0.2060	495.3	3028.6
7	0.2344	512.3	2854.3
8	0.2615	524.6	2716.4
9	0.2865	534.0	2612.4
10	0.3102	540.2	2524.6
11	0.3321	544.0	2452.6
12	0.3569	544.0	2370.3
13	0.3761	545.5	2324.8
14	0.3942	544.0	2278.2
15	0.4119	541.3	2234.7
16	0.4279	537.4	2195.2
17	0.4432	532.9	2159.6
18	0.4578	527.3	2124.3
19	0.4717	521.5	2092.8
20	0.4850	514.9	2061.6
21	0.4972	508.2	2032.8
22	0.5089	502.2	2009.6
23	0.5205	495.0	1983.4
24	0.5268	487.4	1955.4
25	0.5314	487.6	1958.3
26	0.5369	480.8	1933.8
27	0.5420	480.5	1935.5
28	0.5472	473.5	1910.9
29	0.5522	473.8	1916.2
30	0.5576	464.2	1881.7
31	0.5684	456.2	1859.4
32	0.5797	446.9	1834.2
33	0.5915	437.0	1808.8
34	0.6039	426.2	1781.6
35	0.6172	414.4	1753.9
36	0.6306	402.0	1725.8
37	0.6449	388.1	1694.7
38	0.6600	373.4	1664.0
39	0.6758	357.5	1631.9
40	0.6922	341.1	1601.0
41	0.7091	323.4	1567.6
42	0.7268	304.7	1534.5
43	0.7453	283.9	1495.6
44	0.7652	262.7	1462.0
45	0.7856	239.8	1423.8
46	0.8077	215.9	1390.4
47	0.8306	190.0	1350.0
48	0.8547	162.9	1312.1
49	0.8808	134.1	1276.7
50	0.9079	103.4	1237.1
51	0.9367	70.3	1184.5
52	0.9677	35.6	1136.7

TABLE A37:

HEATS OF MIXING OF SYSTEM ISOPENTANOL - N-HEPTANE
TEMP=25 DEG C. DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0217	252.4	11898.2
2	0.0508	353.4	7323.6
3	0.0973	441.2	5025.5
4	0.1395	495.4	4127.0
5	0.1783	534.2	3646.7
6	0.2137	563.1	3351.7
7	0.2463	584.3	3147.7
8	0.2758	600.3	3005.2
9	0.3030	611.8	2896.7
10	0.3286	619.4	2807.8
11	0.3516	624.0	2736.9
12	0.3744	626.1	2673.3
13	0.3950	626.7	2622.5
14	0.4145	624.8	2574.5
15	0.4329	621.8	2532.8
16	0.4501	617.8	2495.9
17	0.4666	612.3	2460.3
18	0.4821	606.3	2428.5
19	0.4966	599.5	2398.3
20	0.5104	592.1	2369.5
21	0.5229	585.2	2345.7
22	0.5351	577.2	2320.4
23	0.5469	570.1	2300.5
24	0.5572	565.3	2291.3
25	0.5578	561.4	2276.2
26	0.5661	558.0	2271.7
27	0.5682	553.0	2254.0
28	0.5762	550.1	2252.7
29	0.5779	545.6	2236.7
30	0.5866	541.2	2231.7
31	0.5970	532.2	2212.0
32	0.6083	521.9	2190.1
33	0.6198	511.0	2168.4
34	0.6320	499.2	2146.3
35	0.6447	486.5	2123.9
36	0.6578	472.4	2098.8
37	0.6715	457.2	2072.6
38	0.6858	442.4	2053.0
39	0.7006	424.8	2025.1
40	0.7158	406.3	1997.3
41	0.7323	386.5	1[illegible]71.6
42	0.7494	364.7	1[illegible]41.9
43	0.7673	341.6	1913.3
44	0.7861	316.5	1882.6
45	0.8053	290.0	1850.1
46	0.8258	261.7	1919.3
47	0.8471	230.9	1783.1
48	0.8697	198.3	1749.8
49	0.8935	163.4	1717.9
50	0.9187	124.5	1667.7
51	0.9442	86.7	1644.9
52	0.9717	43.0	1565.8

TABLE A38:4

HEATS OF MIXING OF SYSTEM ISOPENTANOL - N-OCTANE
TEMP=25 DEG C. DELTA H IN JOULES/MOLE

N	X ALC	DELTA H	DEL H/X1X2
1	0.0247	279.3	11584.2
2	0.0548	383.1	7393.1
3	0.1056	484.1	5127.4
4	0.1513	545.2	4246.4
5	0.1924	588.6	3788.4
6	0.2294	621.2	3514.2
7	0.2647	644.6	3312.5
8	0.2957	661.7	3177.2
9	0.3248	673.8	3072.5
10	0.3524	681.7	2987.3
11	0.3776	686.3	2920.3
12	0.4011	687.7	2862.9
13	0.4228	686.1	2811.4
14	0.4425	683.4	2770.5
15	0.4613	679.7	2735.2
16	0.4784	674.1	2701.5
17	0.4947	667.9	2672.0
18	0.5099	660.9	2644.6
19	0.5269	652.2	2616.5
20	0.5403	643.4	2590.4
21	0.5528	635.4	2570.3
22	0.5645	627.0	2550.6
23	0.5756	618.2	2530.5
24	0.5804	608.6	2499.2
25	0.5866	609.4	2513.0
26	0.5902	600.9	2484.4
27	0.5968	600.6	2495.9
28	0.6002	591.9	2466.8
29	0.6084	590.2	2477.1
30	0.6106	582.4	2449.6
31	0.6214	572.3	2432.8
32	0.6324	561.0	2413.2
33	0.6439	548.8	2393.4
34	0.6559	535.9	2374.2
35	0.6682	522.0	2354.3
36	0.6810	506.9	2333.3
37	0.6944	490.9	2313.2
38	0.7083	473.6	2292.4
39	0.7227	455.3	2271.7
40	0.7375	435.3	2248.4
41	0.7529	414.1	2225.8
42	0.7691	391.6	2205.3
43	0.7858	366.8	2179.1
44	0.8032	340.6	2154.6
45	0.8214	[illegible].7	2131.3
46	0.8404	282.5	2106.0
47	0.8601	250.2	2079.7
48	0.8810	215.2	2052.7
49	0.9029	177.4	2024.0
50	0.9255	137.8	1997.9
51	0.9495	94.5	1969.2
52	0.9743	48.7	1942.9

A3. ALGORITHMS FOR NON-LINEAR PARAMETER ESTIMATION

Let the mathematical model be represented by

$$\eta = f(\underline{\beta}, \underline{x}) \qquad (A3.1)$$

where η is the experimentally observed variable

$\underline{\beta}$ is the vector of unknown k parameters

$\underline{x}$ is the vector of independent variables

The problem is to find an estimate $\underline{b}$ for $\underline{\beta}$ for which the sum of squares

$$\Phi = \sum_{i=1}^{m} (y_i - f_i)^2 \qquad (A3.2)$$

is a minimum where y_i is the ith observation of η and

$f_i = f(\underline{b}, \underline{x}_i)$ where x_i being the corresponding values of the independent variables $\underline{x}$.

The ordinary least-squares method may be applied if the model is expanded in a Taylor Series about a current estimate $\underline{b}_o$, only first order terms being retained. This leads to an improved estimate $\underline{b} = (\underline{b}_o + \underline{t})$ for the linearized model, where $\underline{t}$ is the solution of

$$A \, \underline{t} = \underline{g} \qquad (A3.3)$$

where $A = F'^T F'$ (A3.4)

$\underline{g} = F'^T F$ (A3.5)

$F = (\underline{y} - \underline{f}_o)$ (A3.6)

F' being the (m x k) matrix with elements $\left(\frac{\partial f_i}{\partial b_j}\right)_{\underline{b}=\underline{b}_o}$ and F'^T being the transpose matrix of F'.

If the sum of squares at a new point $\underline{b}$ is smaller than the sum of squares at the point $\underline{b}_o$, then repeated application of this procedure will lead to a solution of the problem. If not, then the Taylor Series method may not converge. However, at points away from the minimum, it is always possible to reduce the sum of squares by taking a sufficiently small step in the direction of steepest descent, $\underline{d}$ (= $-\underline{g}$). Methods based entirely in the direction of steepest descent have not been successful since they take a very large number of iterations.

A3.1 Marquardt's Algorithm

Marquardt's algorithm (M5) is based on the idea that the best direction for finding a reduced sum of squares lies in a direction $\underline{\delta}$ lying between $\underline{d}$ and $\underline{t}$. He finds this direction by solving the equation:

$$(A + \lambda I)\,\underline{\delta} = \underline{g} \qquad \text{(A3.7)}$$

i.e. he adds λ to the diagonal elements of A. (For this to be meaningful, the system must be scaled so that the matrix A has ones on the main diagonal.

When $\lambda = 0$, $\underline{\delta}$ is the Taylor Series direction $\underline{t}$, and as λ increases, $\underline{\delta}$ swings towards the steepest descent direction $\underline{d}$. The idea behind the algorithm is based on the following observations. The method of steepest descent often works well on the initial iterations but the approach to the minimum grows progressively slower. On the other hand, the method of Gauss (Taylor Series) works well when the minimum is near but often gives troubles on the initial iterations. From equation (A3.7), we see that the two extremes are represented by $\lambda \to \infty$ and $\lambda \to 0$.

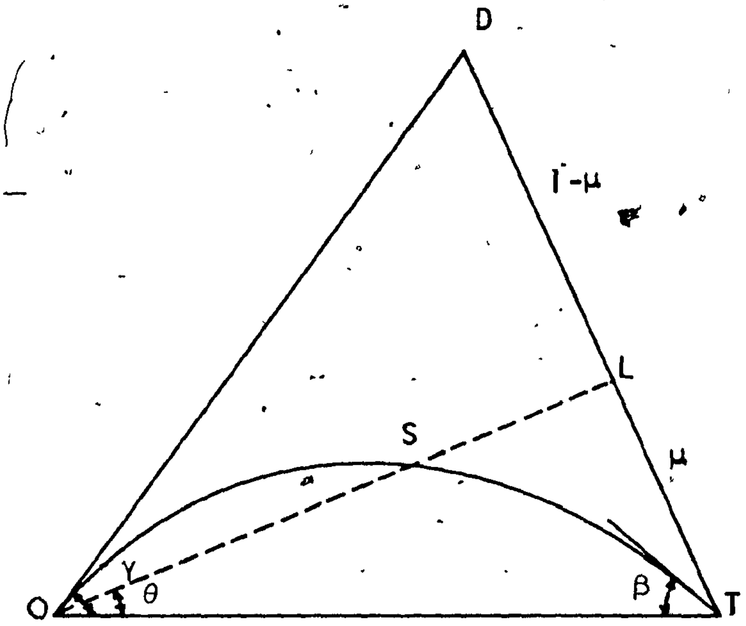
This algorithm should share with the gradient or steepest descent method the ability to converge from a region far from the minimum and like the method of Gauss, should converge rapidly once the vicinity of the minimum is reached. The listing of the Marquardt's program is given in Section A3.3.

A3.2 The Spiral Algorithm

The basic idea behind the Spiral Algorithm (J1-2) is that a reduced sum of squares can always be found in the plane defined by the Taylor Series point and the line of steepest descent at the base point. In Figure A3.1, O is the base

FIGURE A3.1

Geometry of Spiral Algorithm


D
1-μ
L
S
μ
γ
θ
β
O
T

point T is the Taylor Series point and OD is the direction of steepest descent.

Since the sum of squares must decrease initially along OD and since the Taylor Series approximation predicts a reduced sum of squares at the point T, then it is reasonable to assume that the reduced values of the sum of squares can be found in the area OTD.

In the spiral algorithm, a base point for the next iteration is sought as far as possible from the base point O. The first point to be investigated is the Taylor Series point T. It is reasonable to assume that the sum of squares "valley" is moving away from the line OT. To try intercepting the valley, the spiral OTS is searched, this curve moves out from T at an angle β into the area OTD and moves back into O tangentially to OD. The most suitable equation for this spiral (expressed in polar co-ordinates with O as origin) has been found to be

$$r = r_o(1 - \theta \cos \beta - (1 - \gamma \cos \beta)(\theta/\gamma)^2) \quad \text{(A3.8)}$$

where r is the distance OS

r_o is the distance OT

The sequence of points, S, on the spiral to be investigated is computed from a sequence of points, L, generated on the line TD such that L divides TD in the ratio $\mu:(1-\mu)$. The successive values of μ are computed from the recurrence relation:

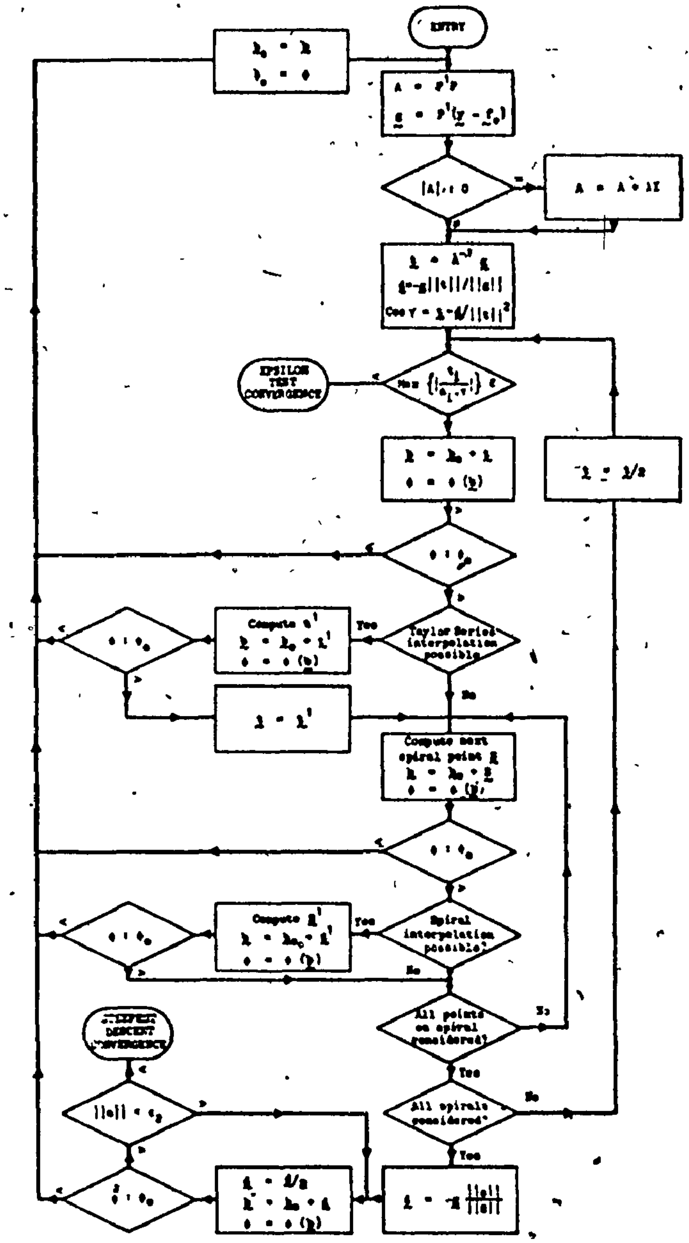
$$\mu_{n+1} = 2\,\mu_n/(1 + \mu_n) \qquad (A3.9)$$

which has chosen to insure that the points become closer together as they approach D.

The above equations are basic for the Spiral Algorithm. A block diagram of the algorithm is given in Figure A3.2. The Spiral program allows, as standard, four spirals to be searched. If a reduced value of the sum of squares has not been found in any of these spirals, then the direction of steepest descent itself is searched. The only occasions that this could happen are for badly defined problems, i.e. problems for which very high correlations exist between parameters. This situation is usually due to redundant parameters in the model, or to poor starting values for parameters.

FIGURE A3.2

Block Diagram of Spiral Algorithm


ENTRY
EPSILON TEST CONVERGENCE
Taylor Series interpolation possible
Yes
No
Compute next spiral point
Spiral interpolation possible?
All points on spiral considered?
All spirals considered?
STEEPEST DESCENT CONVERGENCE

A3.3 Listing of Non-Linear Fitting Program "GAUSS" (Marquardt's Algorithm)

```
G LEVEL  20                      MAIN                 DATE = 71308                  18/12/25

         REAL P(4),H(4),Y(25),G(25),DEV(25)
         REAL DIFZ(4),SIGNS(4)
         COMMON DER,TRACE
         LOGICAL DER
         LOGICAL TRACE
         COMMON/SUB2/XEXP(25),XG(25),YEXP(25),AN1,AN2,V1,V2
         COMMON/SUB3/T
         TRACE=.FALSE.
    1    READ(5,109,END=1000)
  109    FORMAT(1X,79H
        1
        2  /1X,79H
        3
         DER=.TRUE.
         READ(5,110)N,M,I,J,K
  110    FORMAT(5I6)
         M=-M
         READ(5,111)(P(I),I=1,N)
  111    FORMAT(4F10.0)
         READ 901,V1,V2,T,AN1,AN2
  901    FORMAT(5F10.0)
         READ 902,(XEXP(I),YEXP(I),I=1,M)
  902    FORMAT(2F20.0)
         DO 220 I=1,M
         X1=XEXP(I)
         X2=1.-X1
         XC(I)=(AN1*X1+AN2*X2)/((AN1+1.)*X1+AN2*X2)
         YEXP(I)=YEXP(I)*X1*X2
  220    CONTINUE
         EPS1=1.E-07
         EPS2=1.E-07
         NPROB=1
         MIT=40
         FLAM=0.01
         FNU=10.
         DO 10 I=1,N
         DIFZ(I)=0.001
   10    CONTINUE
         SIGNS(1)=1.
         SIGNS(2)=1.
         SIGNS(3)=0.
         SIGNS(4)=0.
         PRINT 25
   25    FORMAT(1H1)
         PRINT 109
         CALL GAUSS(NPROB,M,YEXP,N,P,DIFZ,SIGNS,EPS1,EPS2,MIT,FLAM,FNU)
         GO TO 1
 1000    STOP
         END
```

```
      SUBROUTINE GAUSS(NPROB,NOB,Y,NP,TH,DIFZ,SIGNS,EPS1,EPS2,MIT,
     1                          FLAM,FNU)
      REAL TH(NP),DIFZ(NP),SIGNS(NP),Y(NOB)
      REAL F(25),P(10),PHI(10),Q(10),DELZ(25,10),R(25),TB(10),D(11,11),
     1   E(10),A(11,11)
      LOGICAL DER
      LOGICAL TRACE
      COMMON DER,TRACE
      PRINT 1000, NPROB,NOB,NP
      PRINT 1001
      CALL GAUS60(1,NP,TH,TEMP,TEMP)
      PRINT 1002
      CALL GAUS60(1,NP,DIFZ,TEMP,TEMP)
      IF(NP.LT.1 .OR.NP.GT.50.OR.NOB.LT.NP) GO TO 99
        IF(MIT.LT.1 .OR. MIT.GT.999 .OR. FNU.LT.1.) GO TO 99
      DO 19 I=1,NP
      TEMP = DIFZ(I)
      IF(TEMP) 17,99,18
   17 TEMP=-TEMP
   18 IF(TEMP.GE.1.0 .OR. TH(I).EQ.0.0) GO TO 99
   19 CONTINUE
      GA=FLAM
      NIT=1
      IRAN=1
      JORDAN=1
      IF(EPS1 .LT. 0.0) EPS1=0.0
      IF(EPS2 .GT. 0.0) GO TO 30
      IF(EPS1.GT.0.0) GO TO 50
      IRAN=2
      GO TO 70
   50 IRAN=3
      GO TO 70
   30 IF(EPS1 .GT.0.0) GO TO 70
      JORDAN=2
   70 SSQ=0.0
      CALL FOF(NPROB,TH,F,NOB,NP)
      DO 90 I=1,NOB
      R(I) = Y(I)-F(I)
   90 SSQ= SSQ+R(I)*R(I)
      PRINT 1003, SSQ
C                                                   BEGINE ITERATION
  100 PRINT 1004, NIT
      ICOUNT =0
      GA=GA/FNU
      IF(DER) CALL DERIVE(TH,DELZ,NOB,&122)
      DO 130 J=1,NP
      TEMP=TH(J)
      P(J)=DIFZ(J)*TH(J)
      TH(J)=TH(J)+P(J)
      Q(J)=0.0
      CALL FOF(NPROB,TH,DELZ(1,J),NOB,NP)
      DO 120 I=1,NOB
      DELZ(I,J) = DELZ(I,J)-F(I)
  120 Q(J)=Q(J)+DELZ(I,J)*R(I)
```

```
      Q(J)=Q(J)/P(J)
C                                         Q=XT*R (STEEPEST DESCENT)
  130 TH(J)=TEMP
      GO TO 152
  122 DO 123 J=1,NP
      Q(J)=0.
      DO 123 I=1,NOB
  123 Q(J)=Q(J)+DELZ(I,J)*R(I)
  152 DO 150 I=1,NP
      DO 151 J=1,I
      SUM=0.0
      DO 160 K=1,NOB
  160 SUM=SUM+DELZ(K,I)*DELZ(K,J)
      TEMP=SUM/(P(I)*P(J))
C                                        D=XT*X ( MOMENT MATRIX)
      D(J,I)=TEMP
  151 D(I,J)=TEMP
  150 E(I)=SQRT(D(I,I))
  666 DO 153 I=1,NP
      DO 153 J=1,I
      A(I,J)=D(I,J)/(E(I)*E(J))
      A(J,I)=A(I,J)
  153 CONTINUE
C                                             A=SCALED MOMENT MATRIX
      DO 155 I=1,NP
      P(I) = Q(I)/E(I)
      PHI(I)=P(I)
  155 A(I,I) = A(I,I)+GA
      CALL GAUSS0(NP,A,P,DET,1.0E-30,0,11,&1555,&4100)
 1555 IF(TRACE) PRINT 1005,DET
      STEP=1.0
      SUM1=0.0
      SUM2=0.0
      SUM3=0.0
      DO 231 I=1,NP
      SUM1=SUM1+P(I)*PHI(I)
      SUM2 = SUM2+P(I)*P(I)
      SUM3= SUM3+PHI(I)*PHI(I)
  231 CONTINUE
      ANGLE=SUM1/SQRT(SUM2*SUM3)
      IF(ANGLE.GT.1.0) ANGLE=1.0
      ANGLE=57.295*ARCOS(ANGLE)
      IF(TRACE) PRINT 1041,ANGLE
  170 DO 220 I=1,NP
  220 TB(I)=P(I)*STEP/E(I)+TH(I)
      IF(TRACE) PRINT 7000
 7000 FORMAT(' TEST POINT PARAMETER VALUES')
      IF(TRACE) PRINT 2006,(TB(I),I=1,NP)
      DO 2401 I=1,NP
      IF(SIGNS(I) .GT. 0.0 .AND. TH(I)*TB(I) .LE. 0.0) GO TO 663
 2401 CONTINUE
      SUMB=0.0
      CALL FOF(NPROB,TB,F,NOB,NP)
      DO 230 I=1,NOB
```

```
      R(I)=Y(I)-F(I)
230   SUMB = SUMB+R(I)*R(I)
      IF(TRACE) PRINT 1043,SUMB
      IF(SUMB .LE. SSQ*(1.0+EPS1)) GO TO 662
663   IF(ANGLE.LT.45.0) GO TO 665
      GA=GA*FNU
      ICOUNT= ICOUNT+1
      IF(ICOUNT .GE. 36) GO TO 2700
      GO TO 666
665   STEP=STEP/2.0
      ICOUNT = ICOUNT+1
      IF(ICOUNT .GE. 36) GO TO 2700
      GO TO 170
 662  PRINT 1007
      DO 669 I=1,NP
669   TH(I) = TB(I)
      CALL GAUS60(1,NP,TH,TEMP,TEMP)
      PRINT 1040, GA,SUMB
      GO TO (225,270,265),IRAN
225   HZ=0.0
      HF=0.0
      DO 240 I=1,NP
      HF=HF+ABS(P(I)*STEP/E(I))
      HZ=HZ+ABS(TH(I))
240   CONTINUE
      IF(HF .GT. HZ*EPS2) GO TO 250
      PRINT 1009, EPS2
      GO TO 280
250   GO TO (265,270),JORDAN
265   IF(ABS((SUMB-SSQ)/SSQ) .GT. EPS1) GO TO 270
      PRINT 1010,EPS1
      GO TO 280
270   SSQ=SUMB
      NIT=NIT+1
      IF(NIT.LE.MIT) GO TO 100
      GO TO 280
2700  PRINT 2710
2710  FORMAT(' THE SUM OF SQUARES CANNOT BE REDUCED TO THE SUM OF SQUARES
     1S AT THE END OF THE LAST ITERATION-ITERATING STOPS'/)
C                                        END ITERATION
280   SUM1=0.0
      DO 2714 I=1,NOB
       R(I)=100.*R(I)/Y(I)
2714  SUM1=SUM1+R(I)*R(I)
      RMS=SQRT(SUM1/NOB)
      PRINT 1011,(Y(I),F(I),R(I),I=1,NOB)
      PRINT 1012, RMS
      SSQ=SUMB
      IDF=NOB-NP
      CALL GAUS50(NP,D,P,DET,1.0E-30,-1,11,&7691,&4100)
7691  DO 7692 I=1,NP
 7692 E(I)=SQRT(D(I,I))
      DO 340 I=1,NP
      DO 340 J=I,NP
```

```
      A(I,J) = D(J,I)/(E(I)*E(J))
      D(J,I) = D(J,I)/(DIFZ(I)*TH(I)*DIFZ(J)*TH(J))
      D(I,J) = D(J,I)
340   A(I,J) = A(J,I)
      IF(IDF.EQ.0) GO TO 410
      SDEV=SSQ/IDF
      PRINT 1014, SDEV,IDF
      SDEV = SQRT(SDEV)
      DO 391 I=1,NP
      P(I) = TH(I)+2.0*E(I)*SDEV
391   TB(I) = TH(I)-2.0*E(I)*SDEV
      PRINT 1039
      CALL GAUS60(2,NP,TB,P,TEMP)
      DO 415 K=1,NOB
      TEMP =0.0
      DO 420 I=1,NP
      DO 420 J=1,NP
420   TEMP = TEMP+DELZ(K,I)*DELZ(K,J)*D(I,J)
      TEMP=2.0*SQRT(TEMP)*SDEV
      R(K) = F(K)+TEMP
415   F(K) = F(K)-TEMP
      PRINT 1008
      IE=0
      DO 425 I=1,NOB,10
      IE=IE+10
      IF(NOB .GE. IE) GO TO 435
      IE=NOB
435   PRINT 2001,(R(J),J=1,IE)
425   PRINT 2006,(F(J),J=1,IE)
410   PRINT 1033,NPROB
      RETURN
99    PRINT 1034
      GO TO 410
4100  PRINT 4110
      GO TO 410
1000  FORMAT(1H0,'NONLINEAR ESTIMATION, PROBLEM NUMBER',I3,//I5,'
     1 OBSERVATIONS',I5,'PARAMETERS')
1001  FORMAT(/' INITIAL PARAMETER VALUES')
1002  FORMAT(/' PROPORTIONS USED IN CALCULATING DIFFERENCE QUOTIENTS')
1003  FORMAT(' INITIAL SUM OF SQUARES = ',E12.4)
1004  FORMAT(////45X,'ITERATION NO.',I4)
1005  FORMAT(' DETERMINANT',E12.4)
1006  FORMAT(/' EIGENVALUES OF MOMENT MATRIX-PRELIMINARY ANALYSIS')
1007  FORMAT(/' PARAMETER VALUES VIA REGRESSION')
1008  FORMAT(////' APPROXIMATE CONFIDENCE LIMITS FOR EACH FUNCTION VALUE')
     1')
1009  FORMAT(/' ITERATION STOPS-RELATIVE CHANGE IN EACH PARAMETER LESS T
     1HAN',E12.4)
1010  FORMAT(/' ITERATION STOPS- RELATIVE CHANGE IN SUM OF SQUARES LESS
     1THAN',E12.4)
1011  FORMAT(/T10,'FUNCTION VALUES(EXPTL)',T40,'FUNCTION VALUES(CALD)',T73
     170,'DEVIATION(PCT)',/(T11,E15.7,T41,E15.7,T70,F10.4))
1012  FORMAT(/T50,'RMS DEVIATION(PCT) = ',F10.2)
1014  FORMAT(///' VARIANCE OF RESIDUALS=',E12.4,1H,I4,'DEGREES OF
```

```
V G LEVEL  20                           GAUSS                     DATE = 71308          18/12/25

          1FREEDOM')
    1015   FORMAT(////' CORRELATION MATRIX')
    1016   FORMAT(////' NORMALIZING ELEMENTS')
    1033   FORMAT(//' END OF PROBLEM NO.',I3)
    1034   FORMAT(' ********************PARAMETER ERROR********************')
    1039   FORMAT(/' INDIVIDUAL CONFIDENCE LIMITS FOR EACH PARAMETER(ON LINEAR
          1R HYPOTHESIS)')
    1040   FORMAT(/' LAMDA',E10.3,40X,'SUM OF SQUARES AFTER REGRESSION=',E15.7)
          17)
    1041   FORMAT(' ANGLE IN SCALED COORD.=',F9.2,'DEGREES')
    1043   FORMAT(' TEST POINT SUM OF SQUARES=',E12.4)
    2001   FORMAT(/10E12.4)
    2006   FORMAT(10E12.4)
    4110   FORMAT(5X,' THE MOMENT MATRIX XT*X IS SINGULAR---CONTINUE TO
          1 ANOTHER DATA SET')
           END

S IN EFFECT*  ID,EBCDIC,SOURCE,NOLIST,NODECK,LOAD,NOMAP
S IN EFFECT*  NAME = GAUSS   , LINECNT =       56
TICS*     SOURCE STATEMENTS =      215,PROGRAM SIZE =     10006
TICS*  NO DIAGNOSTICS GENERATED
```

```
      SUBROUTINE GAUS50(N,A,X,DETER,EPS,INDIC,NRC,*,*)
      REAL IROW(10),JCOL(10),JORD(10),Y(10),A(NRC,NRC),X(N)
      MAX=N
      IF(INDIC.LT.0) GO TO 6
      MAX=N+1
      DO 4 I=1,N
    4 A(I,MAX)=X(I)
    6 IF(N.LE.50) GO TO 5
      PRINT 200
      DETER=0.0
      RETURN 2
    5 DETER=1.
      DO 18 K=1,N
      KM1=K-1
      PIVOT=0.0
      DO 11 I=1,N
      DO 11 J=1,N
      IF(K.EQ.1) GO TO 9
      DO 8 ISCAN=1,KM1
      DO 8 JSCAN=1,KM1
      IF(I.EQ.IROW(ISCAN)) GO TO 11
      IF(J.EQ.JCOL(JSCAN)) GO TO 11
    8 CONTINUE
    9 IF(ABS(A(I,J)).LE.ABS(PIVOT)) GO TO 11
      PIVOT=A(I,J)
      IROW(K)=I
      JCOL(K)=J
   11 CONTINUE
      IF(ABS(PIVOT).GT.EPS) GO TO 13
      DETER=0.0
      RETURN 2
   13 IROWK=IROW(K)
      JCOLK=JCOL(K)
      DETER=DETER*PIVOT
      DO 14 J=1,MAX
   14 A(IROWK,J)=A(IROWK,J)/PIVOT
      A(IROWK,JCOLK)=1./PIVOT
      DO 18 I=1,N
      AIJCK=A(I,JCOLK)
      IF(I.EQ.IROWK) GO TO 18
      A(I,JCOLK)=-AIJCK/PIVOT
      DO 17 J=1,MAX
   17 IF(J.NE.JCOLK) A(I,J)=A(I,J)-AIJCK*A(IROWK,J)
   18 CONTINUE
      DO 20 I=1,N
      IROWI=IROW(I)
      JCOLI=JCOL(I)
      JORD(IROWI)=JCOLI
   20 IF(INDIC.GE.0) X(JCOLI)=A(IROWI,MAX)
      INTCH=0
      NM1=N-1
      DO 22 I=1,NM1
      IP1=I+1
      DO 22 J=IP1,N
```

A

```
IV G LEVEL  20                    GAUS50                DATE = 71308              18/1
          IF(JORD(J).GE.JORD(I)) GO TO 22
          JTEMP=JORD(J)
          JORD(J)=JORD(I)
          JORD(I)=JTEMP
          INTCH=INTCH+1
   22     CONTINUE
          IF(INTCH/2*2.NE.INTCH) DETER=-DETER
   24     IF(INDIC.LE.0) GO TO 26
          RETURN 1
   26     DO 28 J=1,N
          DO 27 I=1,N
          IROWI=IROW(I)
          JCOLI=JCOL(I)
   27     Y(JCOLI)=A(IROWI,J)
          DO 28 I=1,N
   28     A(I,J)=Y(I)
          DO 30 I=1,N
          DO 29 J=1,N
          IROWJ=IROW(J)
          JCOLJ=JCOL(J)
   29     Y(IROWJ)=A(I,JCOLJ)
          DO 30 J=1,N.
   30     A(I,J) =Y(J)
          RETURN 1
  200     FORMAT(20X,'**************N IS TOO BIG*****************************'
          END
```

```
:V G LEVEL  20                    GAUS60                DATE = 71308              18/12/25

        SUBROUTINE GAUS60(ITYPE,NP,A,B,C)
        DIMENSION A(NP),B(NP),C(NP,NP)
        DIMENSION IJ(10)
        NR=NP/10
        LOW=1
        LUP=10
  10    IF(NR) 15,20,30
  15    RETURN
  20    LUP=NP
  30    DO 555 J=LOW,LUP
  555   IJ(J)=J
        PRINT 500,(IJ(J),J=LOW,LUP)
        GO TO(40,60,80),ITYPE
  40    PRINT600,(A(J),J=LOW,LUP)
        GO TO 100
  60    PRINT 600,(B(J),J=LOW,LUP)
        GO TO 40
  80    DO 90 I=LOW,LUP
  90    PRINT 720,I,(C(J,I),J=LOW,I)
        IF(NR.EQ.0) RETURN
        LOW2=LUP+1
        DO 95 I=LOW2,NP
  95    PRINT 720,I,(C(J,I),J=LOW,LUP)
  100   LOW=LOW+10
        LUP=LUP+10
        NR=NR-1
        GO TO 10
  500   FORMAT(/I8,9I12)
  600   FORMAT(10E12.4)
  720   FORMAT(1H0,I3,1X,F7.4,9F12.4)
        END
```

```
 G LEVEL  20                      FOF                 DATE = 71308              18/12/25
          SUBROUTINE FOF(NPROB,P,Y,M,NP)
          REAL P(4),Y(25),G(25)
          COMMON/SUB2/XEXP(25),XG(25),YEXP(25),AN1,AN2,V1,V2
          COMMON/SUB3/T
          RT2=1.989*4.18*T*T
          SX1=AN1/(1.+AN1)
          SX2=1.-SX1
          H1S=RT2*(SX2*SX2*P(1)*P(3)/((SX1+SX2*P(1))**2)+SX2*SX2*P(4)/((SX2+
         1SX1*P(2))**2))
          H2S=RT2*(SX1*SX1*P(2)*P(4)/((SX2+SX1*P(2))**2)+SX1*SX1*P(3)/((SX1+
         1SX2*P(1))**2))
          DO 3 I=1,M
          X1=XG(I)
          X2=1.-XG(I)
          H1=RT2*( X2*X2*P(1)*P(3) /(( X1 +X2*P(1))**2)+ X2*X2*P(4)/(( X2+
         1 X1*P(2))**2))
           H2=RT2*( X1* X1*P(2)*P(4)/(( X2+ X1*P(2))**2)+X1* X1*P(3)/(( X1+
         1X2*P(1))**2) )
          G(I)=XEXP(I)*(AN1*(H1-H1S)+H2-H2S)+(1.-XEXP(I))*AN2*H1
        3 Y(I)=G(I)
          RETURN
          END
```

```
      SUBROUTINE DERIVE(P,DFDX,M,*)
      REAL P(4),Y(25),G(25) ,DFDX(25,10)
      COMMON/SUB2/XEXP(25),XG(25),YEXP(25),AN1,AN2,V1,V2
      COMMON/SUB3/T
      SX1=AN1/(1.+AN1)
      SX2=1.-SX1
      RT2=1.989*4.18*T*T
      DH11S=RT2*(SX2*SX2*P(3)*SX1-SX2*SX2*SX2*P(3)*P(1))/((SX1+SX2*P(1))
     1**3)
      DH21S=-RT2*2.*SX1*SX1*SX2*P(3)/((SX1+SX2*P(1))**3)
      DH12S=-RT2*2.*SX2*SX2*SX1*P(4)/((SX2+SX1*P(2))**3)
      DH22S=RT2*(SX1*SX1*SX2*P(4)-SX1*SX1*SX1*P(4)*P(2))/((SX2+SX1*P(2))
     1**3)
      DH13S=RT2*SX2*SX2*P(1)/((SX1+SX2*P(1))**2)
      DH23S=RT2*SX1*SX1/((SX1+SX2*P(1))**2)
      DH14S=RT2*SX2*SX2*1./((SX2+SX1*P(2))**2)
      DH24S=RT2*SX1*SX1*P(2)/((SX2+SX1*P(2))**2)
      DO 1 I=1,M
      X1=XG(I)
      X2=1.-X1
      DH11 =RT2*( X2* X2*P(3)* X1- X2* X2* X2*P(3)*P(1))/(( X1+ X2*P(1))
     1**3)
      DH21 =-RT2*2.*X1*X1*X2*P(3)/(( X1+ X2*P(1))**3)
      DH12 =-RT2*2.* X2* X2* X1*P(4)/(( X2+ X1*P(2))**3)
      DH22 =RT2*( X1* X1* X2*P(4)- X1* X1* X1*P(4)*P(2))/(( X2+ X1*P(2))
     1**3)
      DH13 =RT2* X2* X2*P(1)/(( X1+ X2*P(1))**2)
      DH23 =RT2* X1* X1/(( X1+ X2*P(1))**2)
      DH14 =RT2* X2* X2*1./(( X2+ X1*P(2))**2)
      DH24 =RT2* X1* X1*P(2)/(( X2+ X1*P(2))**2)
      DFDX(I,1)=XEXP(I)*(AN1*(DH11-DH11S)+DH21-DH21S)+(1.-XEXP(I))*AN2*
     1DH11
      DFDX(I,2)=XEXP(I)*(AN1*(DH12-DH12S)+DH22-DH22S)+(1.-XEXP(I))*AN2*
     1DH12
      DFDX(I,3)=XEXP(I)*(AN1*(DH13-DH13S)+DH23-DH23S)+(1.-XEXP(I))*AN2*
     1DH13
      DFDX(I,4)=XEXP(I)*(AN1*(DH14-DH14S)+DH24-DH24S)+(1.-XEXP(I))*AN2*
     1DH14
 1    CONTINUE
      RETURN
      END
```

A4. A Programme for Prediction of Heats of Mixing

```
C     A PROGRAM TO PREDICT HEATS OF MIXING OF ALCOHOL+HYDROCARBON MIXTURES
      DIMENSION TITLE1(20),TITLE2(20)
      DOUBLE PRECISION T
      DOUBLE PRECISION B(4)
      REAL NA,NH,X(60),Y(60),XCH2(60),HCH2(60),HOH(60),DHBH(60),DHBA(60)
      REAL YPRED(60),DEVP(60)
  100 READ(5,101,END=2000) TITLE1,TITLE2
  101 FORMAT(20A4/20A4)
      READ(5,102)N1,N2,N3,N4,N5,N6,N7,N8;N9
  102 FORMAT(5X,9I5)
      READ(5,103)NA,NH,T,LM
  103 FORMAT(3F10.0 ,I5)
      NPTS=N1
      READ(5,107)(X(I),Y(I),I=1,NPTS)
  107 FORMAT(2F20.0)
C     CALCULATION OF STANDARD STATE AND GROUP COMPOSITION
      SX1=NA/(1.+NA)
      SX2=1.-SX1
C     CALCULATION OF WILSON PARAMETERS
      R=8.31439
      B(1)=26.69*DEXP(-1336./T) + 7.705
      B(2)=(26.69)*(1336./T**2)*DEXP(-1336./T)
      B(3)=34.95*DEXP(-2908./T)
      B(4)=(34.95)*(2908./T**2)*DEXP(-2908./T)
      DO 200 I=1,NPTS
  200 XCH2(I)=((X(I)*NA+(1.-X(I))*NH)/((1.+NA)*X(I)+(1.-X(I))*NH))
C     CALCULATION OF DELTAH FROM READ IN DATA
      DO 15 I=1,NPTS
      IF(LM)12,14,12
   14 Y(I)=Y(I)
      GO TO 15
   12 Y(I)=Y(I)*X(I)*(1.-X(I))
   15 CONTINUE
C     CALCULATION OF PREDICTED HEATS OF MIXING
      SHCHA=(SX2*SX2*B(1)*B(2)/((SX1+SX2*B(1))**2)+
     1SX2*SX2*B(4)/((SX2+SX1*B(3))**2))*R*T*T
      SHOHA=(SX1*SX1*B(4)*B(3)/((SX2+SX1*B(3))**2)+
     1SX1*SX1*B(2)/((SX1+SX2*B(1))**2))*R*T*T
      DO 1 I=1,NPTS
      X1=XCH2(I)
      X2=1.-X1
      HCH2(I)=(X2*X2*B(1)*B(2)/((X1+X2*B(1))**2)+X2*X2*B(4)/
     1((X2+X1*B(3))**2))*R*T*T
      HOH(I)=(X1*X1*B(4)*B(3)/((X2+X1*B(3))**2)  +
     1X1*X1*B(2)/((X1+X2*B(1))**2)) *R*T*T
      DHBH(I)=NH*HCH2(I)
      DHBA(I)=(NA*(HCH2(I)-SHCHA) +HOH(I)-SHOHA)
    1 YPRED(I)=X(I)*DHBA(I)+(1.-X(I))*DHBH(I)
C     COMPARISION OF YPRED WITH EXPERIMETAL HEATS OF MIXING
      DI=0.
      DO 320  I=1,NPTS
      DEVP(I)=(Y(I)-YPRED(I))*100./Y(I)
      DI=DI+DEVP(I)**2
  320 CONTINUE
```

```
      FNPTS=NPTS
      ERROR=SQRT(DI/FNPTS)
C     PRINT OUT RESULTS
      PRINT 400
 400  FORMAT(1H1)
      PRINT 410,TITLE1,TITLE2
 410  FORMAT(20A4/20A4)
      PRINT 420,(B(I),I=1,4)
 420  FORMAT(5X,'B(1)=',F10.6,T25,'B(2)=',F10.6/T5 ,'B(3)=',F10.6,
     1 T25,'B(4)=',F10.6)
      PRINT 430
 430  FORMAT(5X,'X',T15,'XCH2',T25,'Y',T35,'YPRED',T45,'DEVP'/)
      PRINT 440,(X(I),XCH2(I),Y(I),YPRED(I),DEVP(I),I=1,NPTS)
 440  FORMAT(2F10.4,3F10.1)
      PRINT 450, ERROR
 450  FORMAT(T40,'RMS DEVIATION=',F10.1)
      GO TO 100
 2000 STOP
      END
```

A5. Prediction Results on Alcohol/Alkane Systems

TABLE A39:

HEATS OF MIXING AT 15 DEG.C. FOR THE SYSTEM N-BUTANOL+N-HEXANE
DELTA H IN JOULES/MOLE .

B(1)= 7.963050 B(2)= 0.004156
B(3)= 0.001440 B(4)= 0.000050

X	XCH2	Y	YPRED	DEVP
0.0272	0.9954	193.8	202.8	-4.7
0.0546	0.9908	257.0	263.3	-2.5
0.1044	0.9823	328.4	333.9	-1.7
0.1479	0.9747	371.8	377.3	-1.5
0.1883	0.9676	402.4	407.3	-1.2
0.2252	0.9610	423.8	427.4	-0.8
0.2582	0.9550	438.0	440.3	-0.5
0.2904	0.9491	446.1	448.6	-0.6
0.3198	0.9437	450.3	452.9	-0.6
0.3478	0.9385	450.9	454.2	-0.7
0.3730	0.9337	448.3	453.2	-1.1
0.3997	0.9286	442.7	450.0	-1.7
0.4203	0.9247	437.8	446.2	-1.9
0.4379	0.9213	432.0	442.0	-2.3
0.4552	0.9179	425.3	437.1	-2.8
0.4727	0.9145	418.0	431.4	-3.2
0.4881	0.9114	410.8	425.8	-3.7
0.5038	0.9083	403.0	419.4	-4.1
0.5207	0.9050	393.6	412.0	-4.7
0.5338	0.9023	386.5	405.8	-5.0
0.5460	0.8999	379.0	399.7	-5.4
0.5559	0.8979	373.0	394.5	-5.8
0.5670	0.8956	365.8	388.4	-6.2
0.5730	0.8944	363.1	385.0	-6.0
0.5767	0.8937	359.8	382.9	-6.4
0.5828	0.8924	356.4	379.4	-6.4
0.5866	0.8916	353.1	377.1	-6.8
0.5927	0.8904	349.6	373.5	-6.8
0.5956	0.8898	347.1	371.7	-7.1
0.6026	0.8884	342.2	367.4	-7.4
0.6130	0.8862	335.0	360.8	-7.7
0.6241	0.8839	327.3	353.5	-8.0
0.6361	0.8814	319.2	345.4	-8.2
0.6479	0.8789	310.7	337.1	-8.5
0.6605	0.8763	301.6	328.1	-8.8
0.6736	0.8735	291.8	318.4	-9.1
0.6870	0.8707	281.5	308.2	-9.5
0.7011	0.8677	270.3	297.1	-9.9
0.7159	0.8645	258.9	285.2	-10.2
0.7313	0.8612	246.6	272.4	-10.5
0.7465	0.8579	233.5	259.5	-11.1
0.7624	0.8544	219.9	245.6	-11.7
0.7797	0.8506	205.8	230.0	-11.8
0.7975	0.8467	190.7	213.6	-12.0
0.8151	0.8428	176.2	197.0	-11.8
0.8338	0.8386	159.6	178.8	-12.0
0.8549	0.8338	141.5	157.9	-11.5
0.8766	0.8289	122.2	135.7	-11.1
0.8990	0.8238	102.3	112.3	-9.8
0.9227	0.8183	81.3	86.9	-6.9
0.9472	0.8125	58.5	60.0	-2.6
0.9729	0.8065	34.4	31.2	9.3

RMS DEVIATION= 7.2

TABLE A40:

HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-BUTANOL+N-HEXANE
DELTA H IN JOULES/MOLE

B(1)= 7.963050 B(2)= 0.004156
B(3)= 0.001440 B(4)= 0.000050

X	XCH2	Y	YPRED	DEVP
0.0272	0.9954	193.8	202.8	-4.7
0.0546	0.9908	257.0	263.3	-2.5
0.1044	0.9823	328.4	333.9	-1.7
0.1479	0.9747	371.8	377.3	-1.5
0.1883	0.9676	402.4	407.3	-1.2
0.2252	0.9610	423.8	427.4	-0.8
0.2582	0.9550	438.0	440.3	-0.5
0.2904	0.9491	446.1	448.6	-0.6
0.3198	0.9437	450.3	452.9	-0.6
0.3478	0.9385	450.9	454.2	-0.7
0.3730	0.9337	448.3	453.2	-1.1
0.3997	0.9286	442.7	450.0	-1.7
0.4203	0.9247	437.8	446.2	-1.9
0.4379	0.9213	432.0	442.0	-2.3
0.4552	0.9179	425.3	437.1	-2.8
0.4727	0.9145	418.0	431.4	-3.2
0.4881	0.9114	410.8	425.8	-3.7
0.5038	0.9083	403.0	419.4	-4.1
0.5207	0.9050	393.6	412.0	-4.7
0.5338	0.9023	386.5	405.8	-5.0
0.5460	0.8999	379.0	399.7	-5.4
0.5559	0.8979	373.0	394.5	-5.8
0.5670	0.8956	365.8	388.4	-6.2
0.5730	0.8944	363.1	385.0	-6.0
0.5767	0.8937	359.8	382.9	-6.4
0.5828	0.8924	356.4	379.4	-6.4
0.5866	0.8916	353.1	377.1	-6.8
0.5927	0.8904	349.6	373.5	-6.8
0.5956	0.8898	347.1	371.7	-7.1
0.6026	0.8884	342.2	367.4	-7.4
0.6130	0.8862	335.0	360.8	-7.7
0.6241	0.8839	327.3	353.5	-8.0
0.6361	0.8814	319.2	345.4	-8.2
0.6479	0.8789	310.7	337.1	-8.5
0.6605	0.8763	301.6	328.1	-8.8
0.6736	0.8735	291.8	318.4	-9.1
0.6870	0.8707	281.5	308.2	-9.5
0.7011	0.8677	270.3	297.1	-9.9
0.7159	0.8645	258.9	285.2	-10.2
0.7313	0.8612	246.6	272.4	-10.5
0.7465	0.8579	233.5	259.5	-11.1
0.7624	0.8544	219.9	245.6	-11.7
0.7797	0.8506	205.8	230.0	-11.8
0.7975	0.8467	190.7	213.6	-12.0
0.8151	0.8428	176.2	197.0	-11.8
0.8338	0.8386	159.6	178.8	-12.0
0.8549	0.8338	141.5	157.9	-11.5
0.8766	0.8289	122.2	135.7	-11.1
0.8990	0.8238	102.3	112.3	-9.8
0.9227	0.8183	81.3	86.9	-6.9
0.9472	0.8125	58.5	60.0	-2.6
0.9729	0.8065	34.4	31.2	9.3

RMS DEVIATION= 7.2

TABLE A41:

```
HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-BUTANOL+N-HEPTANE
DELTA H IN JOULES/MOLE
   B(1)=   7.963050       B(2)=   0.004156
   B(3)=   0.001440       B(4)=   0.000050
    X          XCH2          Y           YPRED       DEVP

  0.0337     0.9951      203.1       241.5      -18.9
  0.0631     0.9908      266.7       304.4      -14.2
  0.1213     0.9820      349.2       384.6      -10.1
  0.1720     0.9742      399.6       432.5       -8.2
  0.2202     0.9664      435.6       464.8       -6.7
  0.2614     0.9596      457.6       483.8       -5.7
  0.2984     0.9534      471.5       494.8       -5.0
  0.3326     0.9475      478.1       500.3       -4.6
  0.3630     0.9421      480.3       501.7       -4.5
  0.3911     0.9371      479.1       500.2       -4.4
  0.4175     0.9323      474.5       496.4       -4.6
  0.4405     0.9280      469.5       491.4       -4.7
  0.4656     0.9233      461.1       484.2       -5.0
  0.4857     0.9194      453.9       477.1       -5.1
  0.5043     0.9158      445.5       469.6       -5.4
  0.5204     0.9127      438.0       462.3       -5.6
  0.5359     0.9096      429.8       454.7       -5.8
  0.5508     0.9066      421.4       446.8       -6.0
  0.5650     0.9037      413.1       438.8       -6.2
  0.5779     0.9011      405.2       431.1       -6.4
  0.5904     0.8985      397.8       423.2       -6.4
  0.5935     0.8979      393.2       421.2       -7.1
  0.6018     0.8962      389.6       415.8       -6.7
  0.6020     0.8961      387.2       415.6       -7.3
  0.6118     0.8941      380.5       409.0       -7.5
  0.6215     0.8920      375.7       402.2       -7.1
  0.6125     0.8939      381.9       408.5       -7.0
  0.6219     0.8920      372.5       401.9       -7.9
  0.6315     0.8899      369.1       394.9       -7.0
  0.6323     0.8898      364.8       394.4       -8.1
  0.6410     0.8879      362.4       387.9       -7.0
  0.6428     0.8875      356.6       386.5       -8.4
  0.6487     0.8862      356.0       382.0       -7.3
  0.6539     0.8851      348.8       378.0       -8.4
  0.6651     0.8827      340.1       369.1       -8.5
  0.6772     0.8800      330.1       359.2       -8.8
  0.6895     0.8773      319.8       348.8       -9.1
  0.7019     0.8746      309.0       338.1       -9.4
  0.7156     0.8715      296.5       325.8       -9.9
  0.7295     0.8683      284.9       313.1       -9.9
  0.7437     0.8651      272.2       299.7      -10.1
  0.7585     0.8617      257.5       285.3      -10.8
  0.7743     0.8580      242.6       269.5      -11.1
  0.7907     0.8541      227.1       252.6      -11.3
  0.8075     0.8500      211.1       234.9      -11.3
  0.8237     0.8461      194.6       217.3      -11.7
  0.8416     0.8417      175.8       197.4      -12.3
  0.8613     0.8368      156.4       174.9      -11.8
  0.8811     0.8318      134.6       151.6      -12.6
  0.9019     0.8264      111.7       126.6      -13.3
  0.9229     0.8209       88.0       100.6      -14.3
  0.9456     0.8149       62.6        71.9      -14.8
  0.9749     0.8070       27.1        33.7      -24.0
                                       RMS DEVIATION=        9.5
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TABLE A42:

```
HEATS OF MIXING AT 15 DEG. C FOR THE SYSTEM N-BUTANOL + N-OCTANE
DELTA H IN JOULES/MOLE
   B(1)=   7.963050      B(2)=   0.004156
  B(3)=  0.001440        B(4)=   0.000050
   X          XCH2        Y           YPRED      DEVP

  0.0352     0.9955      252.3       265.8       -5.4
  0.0680     0.9913      324.2       338.8       -4.5
  0.1266     0.9834      405.8       421.4       -3.8
  0.1787     0.9761      457.5       472.1       -3.2
  0.2265     0.9691      492.3       505.5       -2.7
  0.2687     0.9626      513.8       526.1       -2.4
  0.3074     0.9566      527.4       538.4       -2.1
  0.3430     0.9508      534.1       544.5       -2.0
  0.3749     0.9455      535.7       546.0       -1.9
  0.4030     0.9407      533.9       544.3       -1.9
  0.4286     0.9362      529.2       540.4       -2.1
  0.4531     0.9318      522.9       534.6       -2.3
  0.4745     0.9278      516.2       528.1       -2.3
  0.4950     0.9240      507.7       520.4       -2.5
  0.5128     0.9206      499.2       512.8       -2.7
  0.5300     0.9173      490.2       504.5       -2.9
  0.5442     0.9145      482.0       497.1       -3.1
  0.5580     0.9118      473.8       489.3       -3.3
  0.5718     0.9090      465.2       480.9       -3.4
  0.5844     0.9064      456.6       472.9       -3.6
  0.5969     0.9039      448.3       464.4       -3.6
  0.6092     0.9013      439.0       455.7       -3.8
  0.6122     0.9007      439.4       453.6       -3.2
  0.6206     0.8989      430.2       447.3       -4.0
  0.6212     0.8988      433.0       446.9       -3.2
  0.6304     0.8968      425.9       439.8       -3.3
  0.6310     0.8967      422.1       439.4       -4.1
  0.6399     0.8948      418.0       432.3       -3.4
  0.6412     0.8945      413.9       431.3       -4.2
  0.6496     0.8926      409.7       424.4       -3.6
  0.6512     0.8923      405.4       423.1       -4.4
  0.6602     0.8903      400.7       415.5       -3.7
  0.6709     0.8879      391.5       406.3       -3.8
  0.6823     0.8854      380.6       396.1       -4.1
  0.6944     0.8826      369.9       385.0       -4.1
  0.7061     0.8799      359.4       373.9       -4.0
  0.7189     0.8770      347.0       361.4       -4.1
  0.7323     0.8738      333.7       347.9       -4.3
  0.7454     0.8707      320.3       334.3       -4.3
  0.7593     0.8673      306.1       319.4       -4.3
  0.7735     0.8638      291.2       303.8       -4.3
  0.7887     0.8600      274.8       286.6       -4.3
  0.8045     0.8560      256.5       268.2       -4.6
  0.8212     0.8517      238.6       248.2       -4.0
  0.8373     0.8474      219.5       228.4       -4.1
  0.8547     0.8428      198.5       206.4       -4.0
  0.8728     0.9378      176.1       182.8       -3.8
  0.8921     0.8324      151.6       157.0       -3.6
  0.9123     0.8267      124.9       129.3       -3.5
  0.9335     0.8205       96.8        99.3       -2.6
  0.9558     0.8138       65.9        66.9       -1.4
  0.9782     0.8069       33.0        33.4       -1.3
                                          RMS DEVIATION=        3.5
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TABLE A43:

HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-PENTANOL+N-DECANE
DELTA H IN JOULES/MOLE

B(1)= 7.963050 B(2)= 0.004156
B(3)= 0.001440 B(4)= 0.000050

X	XCH2	Y	YPRED	DEVP
0.0418	0.9957	285.8	317.3	-11.0
0.0665	0.9932	338.8	374.0	-10.4
0.1265	0.9867	427.7	460.3	-7.6
0.1804	0.9806	482.3	511.2	-6.0
0.2293	0.9748	518.3	543.7	-4.9
0.2717	0.9695	545.0	563.2	-3.3
0.3104	0.9646	563.0	574.5	-2.1
0.3445	0.9600	574.9	579.8	-0.8
0.3758	0.9558	581.5	580.9	0.1
0.4047	0.9517	584.0	578.9	0.9
0.4307	0.9480	583.6	574.6	1.5
0.4546	0.9444	580.4	568.7	2.0
0.4754	0.9413	575.4	562.1	2.3
0.4951	0.9383	569.7	554.6	2.6
0.5140	0.9353	561.8	546.3	2.8
0.5306	0.9326	553.7	538.0	2.8
0.5448	0.9303	546.3	530.3	2.9
0.5586	0.9281	539.0	522.3	3.1
0.5733	0.9256	530.1	513.1	3.2
0.5866	0.9234	521.1	504.2	3.2
0.5989	0.9212	511.9	495.6	3.2
0.6100	0.9193	503.4	487.4	3.2
0.6209	0.9174	494.5	479.0	3.1
0.6291	0.9159	481.4	472.5	1.8
0.6309	0.9156	486.0	471.1	3.1
0.6354	0.9148	476.8	467.4	2.0
0.6407	0.9139	477.2	463.0	3.0
0.6434	0.9134	470.1	460.7	2.0
0.6489	0.9124	451.8	456.0	-0.9
0.6527	0.9117	460.8	452.7	1.8
0.6646	0.9095	450.9	442.2	1.9
0.6750	0.9075	441.6	432.7	2.0
0.6859	0.9055	430.7	422.4	1.9
0.6964	0.9035	420.1	412.1	1.9
0.7077	0.9013	408.5	400.8	1.9
0.7198	0.8989	395.7	388.3	1.9
0.7318	0.8965	382.9	375.6	1.9
0.7440	0.8941	368.7	362.2	1.8
0.7572	0.8914	353.7	347.3	1.8
0.7709	0.8885	337.5	331.4	1.8
0.7845	0.8857	321.0	315.2	1.8
0.7983	0.8827	302.9	298.2	1.5
0.8128	0.8796	284.7	279.9	1.7
0.8284	0.8761	263.6	259.7	1.5
0.8450	0.8724	240.7	237.5	1.3
0.8616	0.8685	218.6	214.6	1.8
0.8787	0.8645	194.0	190.4	1.8
0.8979	0.8599	165.6	162.5	1.9
0.9174	0.8551	135.1	133.2	1.4
0.9372	0.8501	103.1	102.6	0.4
0.9570	0.8449	71.8	71.2	0.9
0.9783	0.8393	36.4	36.4	-0.2

RMS DEVIATION= 3.3

TABLE A44:

HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-BUTANOL+N-DECANE
DELTA H IN JOULES/MOLE

B(1)= 7.963050 B(2)= 0.004156
B(3)= 0.001440 B(4)= 0.000050

X	XCH2	Y	YPRED	DEVP
0.0469	0.9952	275.8	338.6	-22.7
0.0766	0.9920	345.6	404.0	-16.9
0.1428	0.9846	448.0	498.8	-11.3
0.2014	0.9776	509.4	555.3	-9.0
0.2531	0.9710	551.1	590.2	-7.1
0.2985	0.9649	577.3	611.0	-5.8
0.3399	0.9591	591.7	622.3	-5.2
0.3756	0.9538	599.9	626.6	-4.5
0.4092	0.9486	601.2	626.2	-4.1
0.4399	0.9436	599.2	622.0	-3.8
0.4661	0.9392	593.8	615.8	-3.7
0.4890	0.9353	587.0	608.3	-3.6
0.5079	0.9319	580.9	600.7	-3.4
0.5279	0.9283	572.2	591.3	-3.3
0.5455	0.9250	563.8	581.9	-3.2
0.5635	0.9215	554.2	571.1	-3.1
0.5821	0.9179	542.5	558.9	-3.0
0.5970	0.9149	533.1	548.2	-2.8
0.6107	0.9121	523.3	537.8	-2.8
0.6225	0.9096	514.4	528.3	-2.7
0.6341	0.9072	505.1	518.6	-2.7
0.6450	0.9048	496.2	509.0	-2.6
0.6551	0.9026	487.4	499.8	-2.5
0.6653	0.9003	479.0	490.1	-2.3
0.6668	0.9000	487.7	488.7	-0.2
0.6748	0.8982	470.5	480.9	-2.2
0.6754	0.8980	479.9	480.3	-0.1
0.6835	0.8962	462.3	472.1	-2.1
0.6840	0.8960	471.6	471.6	0.0
0.6933	0.8939	462.3	462.0	0.1
0.7026	0.8917	452.2	452.1	0.0
0.7123	0.8894	441.6	441.5	0.0
0.7227	0.8868	430.7	429.8	0.2
0.7329	0.8843	418.9	418.0	0.2
0.7431	0.8818	407.2	405.8	0.3
0.7542	0.8789	395.0	392.3	0.7
0.7650	0.8761	381.7	378.7	0.8
0.7759	0.8732	368.6	364.7	1.1
0.7879	0.8700	352.8	348.9	1.1
0.8001	0.8666	337.3	332.3	1.5
0.8125	0.8632	321.0	315.0	1.9
0.8257	0.8594	302.8	296.1	2.2
0.8394	0.8554	283.4	275.9	2.6
0.8531	0.8512	262.9	255.2	2.9
0.8684	0.8465	240.2	231.5	3.6
0.8831	0.8419	217.5	208.0	4.4
0.8980	0.8370	192.4	183.6	4.5
0.9140	0.8317	165.4	156.7	5.2
0.9298	0.8262	137.8	129.4	6.1
0.9468	0.8202	106.5	99.3	6.7
0.9645	0.8137	72.3	67.1	7.2
0.9816	0.8072	38.3	35.2	8.0

RMS DEVIATION= 5.6

TABLE A45:

HEATS OF MIXING AT 15 DEG. C FOR THE SYSTEM N-PENTANOL+N-HEPTANE
DELTA H IN JOULES/MOLE

B(1)= 7.963050   B(2)= 0.004156
B(3)= 0.001440   B(4)= 0.000050

X	XCH2	Y	YPRED	DEVP
0.0315	0.9955	215.2	230.2	-7.0
0.0518	0.9925	261.9	275.3	-5.1
0.1002	0.9855	330.4	344.6	-4.3
0.1435	0.9791	373.0	387.0	-3.7
0.1835	0.9731	403.5	415.9	-3.1
0.2204	0.9675	425.4	435.6	-2.4
0.2542	0.9623	441.9	448.4	-1.5
0.2052	0.9698	362.2	428.2	-18.2
0.3140	0.9530	459.9	460.5	-0.1
0.3384	0.9492	463.4	461.9	0.3
0.3619	0.9455	465.8	461.4	0.9
0.3833	0.9421	463.3	459.6	0.8
0.4019	0.9391	461.0	456.9	0.9
0.4211	0.9360	457.8	453.1	1.0
0.4400	0.9329	452.9	448.4	1.0
0.4568	0.9302	447.4	443.5	0.9
0.4739	0.9274	440.5	437.7	0.6
0.4883	0.9250	434.0	432.3	0.4
0.5054	0.9222	426.2	425.3	0.2
0.5172	0.9202	419.8	420.1	-0.1
0.5284	0.9184	413.7	414.9	-0.3
0.5407	0.9163	407.0	408.8	-0.4
0.5525	0.9143	400.0	402.6	-0.7
0.5570	0.9135	399.7	400.2	-0.1
0.5639	0.9124	393.2	396.5	-0.8
0.5668	0.9119	393.4	394.8	-0.4
0.5747	0.9106	386.4	390.3	-1.0
0.5769	0.9102	386.4	389.1	-0.7
0.5849	0.9088	379.2	384.3	-1.3
0.5877	0.9083	378.5	382.7	-1.1
0.5986	0.9065	370.5	376.0	-1.5
0.6102	0.9045	361.8	368.6	-1.9
0.6222	0.9024	352.8	360.7	-2.2
0.6341	0.9004	343.4	352.6	-2.7
0.6472	0.8981	333.1	343.4	-3.1
0.6605	0.8958	321.8	333.8	-3.7
0.6739	0.8935	310.3	323.8	-4.3
0.6882	0.8910	298.3	312.8	-4.9
0.7027	0.8884	285.6	301.2	-5.5
0.7179	0.8857	272.0	288.8	-6.2
0.7334	0.8830	257.7	275.7	-7.0
0.7504	0.8799	241.8	260.9	-7.9
0.7679	0.8768	225.8	245.3	-8.6
0.7867	0.8734	207.6	228.0	-9.8
0.8063	0.8698	189.6	209.4	-10.5
0.8269	0.8660	169.0	189.4	-12.0
0.8485	0.8621	148.3	167.7	-13.1
0.8704	0.8580	127.0	145.1	-14.3
0.8941	0.8536	102.9	120.0	-16.6
0.9162	0.8494	81.1	96.0	-18.5
0.9424	0.8444	54.3	66.8	-23.0
0.9722	0.8387	25.3	32.7	-29.4

RMS DEVIATION= 8.3

TABLE A46:

HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-HEXANOL+N-HEPTANE
DELTA H IN JOULES/MOLE

B(1)= 7.963050 B(2)= 0.004156
B(3)= 0.001440 B(4)= 0.000050

X	XCH2	Y	YPRED	DEVP
0.0280	0.9960	210.8	216.1	-2.5
0.0455	0.9935	248.5	256.9	-3.4
0.0885	0.9874	307.6	319.1	-3.8
0.1276	0.9818	343.8	357.1	-3.9
0.1642	0.9765	369.3	383.3	-3.8
0.1961	0.9720	387.8	400.6	-3.3
0.2260	0.9677	402.8	412.7	-2.4
0.2531	0.9638	412.5	420.6	-2.0
0.2773	0.9604	420.2	425.5	-1.2
0.3008	0.9570	426.3	428.3	-0.5
0.3231	0.9538	430.2	429.4	0.2
0.3438	0.9509	432.5	429.0	0.8
0.3632	0.9481	433.2	427.6	1.3
0.3812	0.9455	432.6	425.4	1.7
0.3997	0.9429	431.2	422.3	2.1
0.4169	0.9404	429.3	418.6	2.5
0.4360	0.9377	426.2	413.7	2.9
0.4519	0.9354	421.3	409.0	2.9
0.4659	0.9334	416.8	404.4	3.0
0.4789	0.9316	411.8	399.8	2.9
0.4908	0.9299	406.9	395.2	2.9
0.5017	0.9283	402.2	390.8	2.8
0.5139	0.9266	396.9	385.6	2.9
0.5216	0.9255	390.3	382.1	2.1
0.5256	0.9249	391.7	380.3	2.9
0.5318	0.9240	384.7	377.4	1.9
0.5366	0.9233	386.4	375.1	2.9
0.5416	0.9226	379.1	372.6	1.7
0.5488	0.9216	379.1	369.0	2.7
0.5527	0.9210	373.1	367.0	1.6
0.5640	0.9194	366.2	361.1	1.4
0.5763	0.9177	358.0	354.5	1.0
0.5887	0.9159	349.9	347.5	0.7
0.6012	0.9141	341.2	340.2	0.3
0.6145	0.9122	331.6	332.1	-0.1
0.6284	0.9102	322.0	323.4	-0.4
0.6418	0.9083	311.7	314.7	-0.9
0.6567	0.9062	299.8	304.7	-1.6
0.6731	0.9038	286.7	293.4	-2.3
0.6890	0.9016	274.1	282.0	-2.9
0.7067	0.8990	258.5	268.9	-4.0
0.7255	0.8964	241.6	254.6	-5.4
0.7446	0.8936	244.0	239.6	1.8
0.7647	0.8908	206.9	223.2	-7.9
0.7863	0.8877	188.2	205.2	-9.0
0.8049	0.8850	171.5	189.2	-10.3
0.8287	0.8816	149.5	168.1	-12.5
0.8536	0.8781	126.6	145.5	-14.9
0.8792	0.8744	102.9	121.5	-18.1
0.9070	0.8704	77.2	94.7	-22.8
0.9354	0.8664	52.7	66.6	-26.5
0.9636	0.8623	26.8	38.0	-41.8

RMS DEVIATION= 9.0

TABLE A47:

HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-HEXANOL+N-OCTANE
DELTA H IN JOULES/MOLE

B(1)= 7.963050   B(2)= 0.004156
B(3)= 0.001440   B(4)= 0.000050

X	XCH2	Y	YPRED	DEVP
0.0232	0.9971	203.8	217.0	-6.5
0.0503	0.9937	270.9	289.1	-6.7
0.0977	0.9876	337.6	357.7	-6.0
0.1409	0.9821	377.9	398.9	-5.6
0.1795	0.9770	406.1	425.8	-4.9
0.2164	0.9722	427.8	444.7	-3.9
0.2493	0.9678	443.7	456.7	-2.9
0.2797	0.9638	454.9	464.1	-2.0
0.3080	0.9600	462.5	468.0	-1.2
0.3318	0.9567	466.3	469.4	-0.7
0.3529	0.9539	468.1	469.1	-0.2
0.3746	0.9509	470.2	467.4	0.6
0.3953	0.9480	470.2	464.5	1.2
0.4152	0.9453	468.6	460.7	1.7
0.4337	0.9427	465.7	456.1	2.0
0.4503	0.9404	462.4	451.4	2.4
0.4666	0.9381	457.7	446.0	2.6
0.4810	0.9360	452.8	440.7	2.7
0.4945	0.9341	447.7	435.3	2.8
0.5067	0.9324	442.4	430.1	2.8
0.5177	0.9308	437.2	425.1	2.8
0.5287	0.9292	432.3	419.9	2.9
0.5404	0.9276	426.4	414.0	2.9
0.5497	0.9262	419.1	409.2	2.4
0.5516	0.9259	420.7	408.1	3.0
0.5593	0.9248	414.3	403.9	2.5
0.5642	0.9241	413.1	401.2	2.9
0.5694	0.9234	407.5	398.2	2.3
0.5748	0.9226	406.4	395.1	2.8
0.5798	0.9219	400.8	392.2	2.1
0.5914	0.9202	392.4	385.1	1.9
0.6028	0.9185	385.0	378.0	1.8
0.6142	0.9168	376.5	370.6	1.6
0.6261	0.9151	367.1	362.6	1.2
0.6386	0.9133	357.5	353.9	1.0
0.6517	0.9113	346.6	344.5	0.6
0.6648	0.9094	334.9	334.8	0.0
0.6793	0.9072	322.9	323.7	-0.3
0.6945	0.9049	309.8	311.7	-0.6
0.7098	0.9026	294.8	299.3	-1.5
0.7250	0.9003	280.5	286.5	-2.1
0.7421	0.8978	264.1	271.8	-2.9
0.7593	0.8951	247.8	256.4	-3.5
0.7783	0.8922	229.1	239.0	-4.3
0.7973	0.8893	209.1	221.0	-5.7
0.8187	0.8860	186.7	200.2	-7.2
0.8387	0.8829	166.0	180.1	-8.5
0.8623	0.8792	141.4	155.8	-10.2
0.8867	0.8753	115.4	129.8	-12.5
0.9114	0.8714	89.8	102.8	-14.5
0.9397	0.8669	59.9	71.0	-18.5
0.9681	0.8623	29.3	38.1	-29.8

RMS DEVIATION= 6.6

TABLE A48:

```
HEATS OF MIXING AT 15 DEG C FOR THE SYSTEM N-OCTANOL+N-HEXANE
DELTA H IN JOULES/MOLE
    B(1)=   7.963050    B(2)=   0.004156
    B(3)=  0.001440     B(4)=   0.000050
     X         XCH2        Y           YPRED      DEVP

    0.0171     0.9972      160.7       157.9        1.7
    0.0316     0.9948      199.0       198.3        0.4
    0.0627     0.9899      244.2       245.8       -0.6
    0.0925     0.9853      271.7       275.0       -1.2
    0.1185     0.9814      289.6       294.0       -1.5
    0.1431     0.9777      303.6       308.1       -1.5
    0.1679     0.9742      315.5       319.2       -1.2
    0.1923     0.9708      325.2       327.5       -0.7
    0.2144     0.9677      331.8       333.1       -0.4
    0.2334     0.9652      336.9       336.6        0.1
    0.2513     0.9628      341.1       338.9        0.7
    0.2690     0.9605      344.9       340.2        1.4
    0.2861     0.9583      347.2       340.7        1.9
    0.3014     0.9563      349.3       340.5        2.5
    0.3165     0.9545      350.9       339.8        3.2
    0.3321     0.9525      351.8       338.5        3.8
    0.3474     0.9507      352.1       336.7        4.4
    0.3619     0.9489      351.7       334.6        4.9
    0.3753     0.9473      351.2       332.3        5.4
    0.3880     0.9458      350.2       329.8        5.8
    0.4012     0.9443      348.6       326.9        6.2
    0.4128     0.9430      346.6       324.1        6.5
    0.4239     0.9417      344.3       321.2        6.7
    0.4342     0.9405      342.2       318.3        7.0
    0.4446     0.9394      339.8       315.3        7.2
    0.4523     0.9385      337.6       312.9        7.3
    0.4628     0.9374      326.2       309.6        5.1
    0.4719     0.9364      324.7       306.6        5.6
    0.4820     0.9353      322.3       303.1        6.0
    0.4924     0.9341      318.7       299.3        6.1
    0.5033     0.9330      315.2       295.3        6.3
    0.5156     0.9317      310.4       290.5        6.4
    0.5280     0.9304      305.8       285.5        6.6
    0.5410     0.9290      300.0       280.1        6.6
    0.5547     0.9276      293.9       274.1        6.7
    0.5682     0.9263      287.8       268.1        6.8
    0.5832     0.9247      280.3       261.1        6.8
    0.5995     0.9231      271.1       253.3        6.5
    0.6166     0.9215      260.3       244.9        5.9
    0.6344     0.9197      251.0       235.8        6.0
    0.6534     0.9179      239.2       225.7        5.6
    0.6726     0.9161      227.0       215.3        5.2
    0.6931     0.9142      213.1       203.8        4.4
    0.7151     0.9122      198.2       191.1        3.6
    0.7379     0.9102      182.2       177.6        2.5
    0.7627     0.9080      164.9       162.5        1.4
    0.7896     0.9056      144.7       145.6       -0.6
    0.8182     0.9032      124.5       127.2       -2.2
    0.8494     0.9006      102.0       106.6       -4.5
    0.8831     0.8979       76.9        83.7       -8.8
    0.9198     0.8950       50.6        58.1      -14.8
    0.9564     0.8922       24.9        31.9      -28.1
                                          RMS DEVIATION=        6.5
```

TABLE A49:

HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-OCTANOL+N-HEPTANE
DELTA H IN JOULES/MOLE

B(1)= 7.963050 B(2)= 0.004156
B(3)= 0.001440 B(4)= 0.000050

X	XCH2	Y	YPRED	DEVP
0.0208	0.9970	188.3	187.1	0.7
0.0352	0.9950	224.4	226.9	-1.1
0.0699	0.9902	276.4	280.9	-1.6
0.1017	0.9859	307.2	312.2	-1.6
0.1316	0.9819	328.3	333.9	-1.7
0.1598	0.9782	344.3	349.5	-1.5
0.1854	0.9748	355.8	360.4	-1.3
0.2076	0.9720	363.9	367.6	-1.0
0.2278	0.9694	370.8	372.6	-0.5
0.2484	0.9669	376.6	376.3	0.1
0.2686	0.9644	381.5	378.6	0.8
0.2883	0.9619	385.3	379.7	1.5
0.3063	0.9598	388.0	379.8	2.1
0.3234	0.9577	389.9	379.1	2.8
0.3383	0.9559	390.6	377.9	3.3
0.3532	0.9542	390.9	376.2	3.8
0.3675	0.9525	391.4	374.1	4.4
0.3823	0.9508	390.8	371.5	5.0
0.3960	0.9492	389.9	368.6	5.4
0.4094	0.9476	388.6	365.5	5.9
0.4223	0.9462	386.4	362.1	6.3
0.4341	0.9448	384.5	358.8	6.7
0.4450	0.9436	382.1	355.5	6.9
0.4553	0.9424	379.9	352.2	7.3
0.4583	0.9421	382.6	351.2	8.2
0.4665	0.9412	376.3	348.4	7.4
0.4678	0.9411	380.9	348.0	8.7
0.4750	0.9403	373.6	345.4	7.5
0.4778	0.9399	378.3	344.4	9.0
0.4880	0.9388	373.8	340.6	8.9
0.5012	0.9374	370.5	335.4	9.5
0.5136	0.9360	366.2	330.2	9.8
0.5263	0.9346	360.3	324.8	9.8
0.5392	0.9333	354.8	319.0	10.1
0.5528	0.9318	348.6	312.6	10.3
0.5673	0.9303	341.0	305.6	10.4
0.5816	0.9288	333.1	298.4	10.4
0.5978	0.9271	323.6	289.9	10.4
0.6150	0.9253	313.5	280.5	10.5
0.6326	0.9235	301.7	270.6	10.3
0.6503	0.9217	290.6	260.3	10.4
0.6698	0.9197	277.1	248.5	10.3
0.6913	0.9175	261.6	235.1	10.2
0.7147	0.9152	243.3	219.9	9.6
0.7395	0.9128	224.8	203.3	9.6
0.7656	0.9103	188.1	185.2	1.5
0.7941	0.9075	164.3	164.8	-0.3
0.8242	0.9047	140.3	142.6	-1.7
0.8547	0.9019	114.9	119.3	-3.9
0.8869	0.8989	87.9	94.1	-7.0
0.9244	0.8955	57.7	63.8	-10.6
0.9581	0.8925	28.9	35.8	-23.7

RMS DEVIATION= 7.6

TABLE A50:

```
HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-OCTANOL+N-OCTANE
DELTA H IN JOULES/MOLE
    B(1)=  7.963050     B(2)=   0.004156
   B(3)=  0.001440      B(4)=   0.000050
    X          XCH2       Y              YPRED      DEVP

    0.0201     0.9975     192.3          199.1        -3.6
    0.0378     0.9953     241.7          253.2        -4.7
    0.0741     0.9908     297.1          312.0        -5.0
    0.1096     0.9865     332.3          347.6        -4.6
    0.1418     0.9826     355.1          371.0        -4.5
    0.1705     0.9791     371.4          386.8        -4.1
    0.1966     0.9760     382.6          397.8        -4.0
    0.2205     0.9732     391.9          405.5        -3.5
    0.2437     0.9704     399.6          410.9        -2.8
    0.2661     0.9678     405.8          414.4        -2.1
    0.2872     0.9653     410.7          416.3        -1.4
    0.3068     0.9631     414.7          416.9        -0.5
    0.3262     0.9608     417.2          416.4         0.2
    0.3437     0.9588     418.4          415.2         0.8
    0.3607     0.9569     418.3          413.2         1.2
    0.3757     0.9551     418.0          410.9         1.7
    0.3905     0.9535     417.7          408.1         2.3
    0.4048     0.9518     416.8          404.9         2.9
    0.4197     0.9502     415.5          401.1         3.5
    0.4336     0.9486     413.6          397.2         4.0
    0.4470     0.9471     411.3          393.0         4.4
    0.4618     0.9454     407.1          388.0         4.7
    0.4723     0.9443     404.3          384.2         5.0
    0.4837     0.9430     400.8          379.9         5.2
    0.4909     0.9422     396.6          377.0         4.9
    0.4942     0.9418     397.4          375.7         5.5
    0.5003     0.9411     393.7          373.1         5.2
    0.5048     0.9406     393.0          371.2         5.5
    0.5099     0.9401     390.6          369.0         5.5
    0.5203     0.9389     386.6          364.3         5.8
    0.5308     0.9378     381.8          359.4         5.9
    0.5420     0.9365     376.6          354.0         6.0
    0.5536     0.9353     370.7          348.2         6.1
    0.5664     0.9339     364.2          341.6         6.2
    0.5793     0.9325     356.8          334.6         6.2
    0.5936     0.9309     348.8          326.6         6.4
    0.6081     0.9294     339.8          318.2         6.4
    0.6239     0.9277     329.4          308.6         6.3
    0.6405     0.9259     317.3          298.3         6.0
    0.6586     0.9239     304.2          286.6         5.8
    0.6767     0.9220     289.9          274.4         5.3
    0.6964     0.9199     273.8          260.8         4.8
    0.7177     0.9177     256.1          245.5         4.1
    0.7391     0.9154     237.6          229.6         3.4
    0.7620     0.9130     217.4          212.0         2.5
    0.7848     0.9107     196.9          194.0         1.5
    0.8077     0.9083     175.4          175.3         0.0
    0.8352     0.9055     150.1          152.2        -1.4
    0.8638     0.9025     123.8          127.5        -3.0
    0.8945     0.8994      95.1          100.1        -5.2
    0.9289     0.8960      63.1           68.4        -8.5
    0.9609     0.8928      33.0           38.1       -15.4
                                          RMS DEVIATION=        5.0
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TABLE A51:

```
HEATS OF MIXING AT 15 DEG.C FOR THE SYSTEM N-OCTANOL+N-DECANE
DELTA H IN JOULES/MOLE
   B(1)=   7.963050      B(2)=   0.004156
  B(3)=  0.001440      B(4)=   0.000050
   X           XCH2        Y          YPRED.      DEVP

  0.0234      0.9977      221.6      240.7       -8.6
  0.0447      0.9955      278.5      308.7      -10.9
  0.0891      0.9910      346.2      380.7      -10.0
  0.1298      0.9868      385.4      420.2       -9.0
  0.1654      0.9832      410.3      444.6       -8.4
  0.1981      0.9798      429.2      461.1       -7.4
  0.2261      0.9769      440.9      471.5       -6.9
  0.25[illegible]2      0.9740      452.3      478.7       -5.8
  0.2803      0.9712      460.2      483.4       -5.0
  0.3056      0.9685      466.9      485.5       -4.0
  0.3282      0.9661      471.0      485.8       -3.1
  0.3494      0.9638      474.0      484.6       -2.3
  0.3701      0.9616      474.6      482.3       -1.6
  0.3884      0.9596      475.3      479.3       -0.8
  0.4062      0.9577      475.2      475.5       -0.1
  0.4235      0.9558      473.9      471.1        0.6
  0.4400      0.9540      472.1      466.2        1.2
  0.4559      0.9522      469.6      460.9        1.8
  0.4707      0.9506      466.1      455.4        2.3
  0.4841      0.9491      463.0      450.0        2.8
  0.4968      0.9477      459.7      444.5        3.3
  0.5095      0.9463      455.3      438.7        3.7
  0.5213      0.9450      450.9      433.0        4.0
  0.5322      0.9438      446.9      427.4        4.4
  0.5428      0.9426      442.2      421.8        4.6
  0.5430      0.9426      447.9      421.7        5.9
  0.5529      0.9415      437.1      416.2        4.8
  0.5535      0.9414      443.6      415.9        6.3
  0.5642      0.9402      437.7      409.7        6.4
  0.5747      0.9390      431.2      403.5        6.4
  0.5853      0.9378      424.3      397.0        6.4
  0.5963      0.9366      416.7      390.0        6.4
  0.6077      0.9353      409.3      382.5        6.6
  0.6194      0.9340      401.2      374.5        6.7
  0.6316      0.9326      393.2      366.0        6.9
  0.6464      0.9309      381.9      355.3        7.0
  0.6615      0.9292      369.9      343.9        7.0
  0.6764      0.9275      357.4      332.4        7.0
  0.6907      0.9258      344.8      320.9        6.9
  0.7106      0.9235      326.0      304.4        6.6
  0.7288      0.9214      310.5      288.9        7.0
  0.7450      0.9195      293.3      274.4        6.4
  0.7638      0.9173      274.6      257.2        6.3
  0.7881      0.9144      248.7      234.3        5.8
  0.8093      0.9119      225.3      213.5        5.2
  0.8306      0.9094      200.8      192.0        4.4
  0.8553      0.9065      173.5      166.3        4.2
  0.8796      0.9036      145.4      140.2        3.6
  0.9042      0.9006      114.1      113.0        0.9
  0.9347      0.8969       75.4       78.2       -3.7
  0.9615      0.8936       42.2       46.7      -10.7
                                       RMS DEVIATION=        5.8
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TABLE A52:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-BUTANOL+N-HEPTANE
DELTA H IN JOULES/MOLE
    B(1)=  8.159353     B(2)=  0.005642
   B(3)=  0.004932      B(4)=  0.000133
    X           XCH2        Y           YPRED       DEVP

   0.0305      0.9956      493.0       472.8        4.1
   0.0617      0.9910      702.6       684.8        2.5
   0.1159      0.9829      885.0       883.8        0.1
   0.1648      0.9753      980.3       988.0       -0.8
   0.2091      0.9682     1038.2      1048.1       -1.0
   0.2490      0.9617     1073.6      1082.1       -0.8
   0.2860      0.9555     1094.3      1099.7       -0.5
   0.3192      0.9498     1104.8      1105.5       -0.1
   0.3492      0.9446     1107.2      1103.6        0.3
   0.3770      0.9396     1103.9      1096.1        0.7
   0.4026      0.9350     1095.5      1084.8        1.0
   0.4252      0.9309     1087.1      1071.5        1.4
   0.4465      0.9269     1074.6      1056.2        1.7
   0.4657      0.9233     1061.0      1040.2        2.0
   0.4847      0.9196     1046.0      1022.5        2.2
   0.5024      0.9162     1030.2      1004.4        2.5
   0.5189      0.9130     1013.8       986.0        2.7
   0.5345      0.9099      996.7       967.5        2.9
   0.5491      0.9070      979.7       949.1        3.1
   0.5625      0.9043      963.0       931.4        3.3
   0.5749      0.9017      946.5       914.3        3.4
   0.5863      0.8994      930.7       898.0        3.5
   0.5979      0.8970      904.7       880.8        2.6
   0.5996      0.8966      911.3       878.2        3.6
   0.6076      0.8950      890.5       866.0        2.8
   0.6090      0.8947      897.2       863.8        3.7
   0.6173      0.8929      875.0       850.8        2.8
   0.6180      0.8928      883.6       849.7        3.8
   0.6272      0.8908      859.1       834.9        2.8
   0.6280      0.8907      867.9       833.6        3.9
   0.6373      0.8887      841.1       818.3        2.7
   0.6476      0.8865      826.6       801.0        3.1
   0.6585      0.8841      808.0       782.2        3.2
   0.6697      0.8817      787.7       762.4        3.2
   0.6813      0.8791      767.3       741.4        3.4
   0.6933      0.8765      744.2       719.2        3.4
   0.7057      0.8737      720.5       695.7        3.4
   0.7186      0.8708      694.2       670.7        3.4
   0.7321      0.8678      666.6       643.9        3.4
   0.7462      0.8645      636.9       615.2        3.4
   0.7637      0.8605      601.1       578.8        3.7
   0.7790      0.8569      567.4       546.1        3.8
   0.7949      0.8531      532.0       511.4        3.9
   0.8114      0.8491      493.4       474.5        3.8
   0.8288      0.8449      450.8       434.8        3.5
   0.8463      0.8405      408.0       393.9        3.5
   0.8657      0.8357      363.8       347.6        4.4
   0.8856      0.8306      312.8       299.0        4.4
   0.9065      0.8252      257.5       246.9        4.1
   0.9284      0.8195      199.4       191.0        4.2
   0.9514      0.8133      136.6       131.0        4.1
   0.9752      0.8069       70.8        67.5        4.6
                                     RMS DEVIATION=         3.1
```

TABLE A53:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-BUTANOL+N-OCTANE
DELTA H IN JOULES/MOLE

B(1)= 8.159353 B(2)= 0.005642
B(3)= 0.004932 B(4)= 0.000133

X	XCH2	Y	YPRED	DEVP
0.0338	0.9957	539.8	529.6	1.9
0.0708	0.9909	778.6	780.3	-0.2
0.1301	0.9829	970.4	993.1	-2.3
0.1820	0.9756	1066.1	1099.9	-3.2
0.2288	0.9687	1123.1	1160.0	-3.3
0.2705	0.9624	1157.1	1192.0	-3.0
0.3074	0.9566	1175.7	1206.2	-2.6
0.3417	0.9510	1183.2	1209.0	-2.2
0.3721	0.9459	1183.9	1203.8	-1.7
0.4001	0.9412	1178.3	1193.1	-1.3
0.4254	0.9367	1170.4	1178.9	-0.7
0.4488	0.9325	1158.0	1162.1	-0.4
0.4699	0.9287	1144.1	1144.0	0.0
0.4896	0.9250	1128.5	1124.7	0.3
0.5072	0.9217	1113.0	1105.6	0.7
0.5234	0.9186	1097.1	1086.5	1.0
0.5393	0.9155	1080.5	1066.3	1.3
0.5550	0.9124	1061.5	1045.1	1.5
0.5691	0.9096	1043.9	1025.0	1.8
0.5822	0.9069	1026.5	1005.3	2.1
0.5945	0.9044	1008.9	986.1	2.3
0.6087	0.9014	987.0	963.0	2.4
0.6178	0.8995	973.5	947.7	2.7
0.6230	0.8984	949.1	938.8	1.1
0.6280	0.8973	957.1	930.1	2.8
0.6324	0.8964	933.8	922.3	1.2
0.6381	0.8951	940.3	912.2	3.0
0.6420	0.8943	917.0	905.1	1.3
0.6473	0.8932	924.6	895.4	3.2
0.6519	0.8921	900.2	886.9	1.5
0.6565	0.8911	908.6	878.3	3.3
0.6620	0.8899	882.0	867.9	1.6
0.6724	0.8876	862.2	847.8	1.7
0.6836	0.8851	840.7	825.6	1.8
0.6948	0.8825	818.5	802.9	1.9
0.7067	0.8798	794.7	778.2	2.1
0.7187	0.8770	769.3	752.7	2.2
0.7308	0.8742	743.3	726.3	2.3
0.7435	0.8711	715.2	698.0	2.4
0.7567	0.8679	685.6	667.9	2.6
0.7705	0.8646	653.0	635.7	2.6
0.7839	0.8612	621.2	603.8	2.8
0.7984	0.8576	585.7	568.4	3.0
0.8133	0.8537	547.2	531.2	2.9
0.8291	0.8496	506.8	490.9	3.1
0.8452	0.8453	464.2	448.9	3.3
0.8620	0.8408	418.1	404.0	3.4
0.8796	0.8359	369.4	356.0	3.6
0.8978	0.8308	316.8	305.2	3.7
0.9169	0.8253	260.4	250.7	3.7
0.9369	0.8195	200.0	192.4	3.8
0.9568	0.8135	138.6	133.0	4.0
0.9786	0.8068	69.2	66.6	3.7

RMS DEVIATION= 2.5

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-BUTANOL+N-NONANE
DELTA H IN JOULES/MOLE

B(1)= 8.159353 B(2)= 0.005642
B(3)= 0.004932 B(4)= 0.000133

X	XCH2	Y	YPRED	DEVP
0.0361	0.9959	578.9	576.5	0.4
0.0719	0.9917	821.5	833.8	-1.5
0.1347	0.9841	1031.4	1074.9	-4.2
0.1900	0.9769	1137.2	1193.8	-5.0
0.2391	0.9703	1197.5	1258.3	-5.1
0.2829	0.9640	1231.8	1291.6	-4.9
0.3219	0.9583	1249.4	1305.3	-4.5
0.3575	0.9528	1256.0	1306.2	-4.0
0.3900	0.9476	1254.0	1298.2	-3.5
0.4189	0.9428	1246.3	1284.3	-3.1
0.4456	0.9383	1234.5	1266.3	-2.6
0.4697	0.9340	1219.5	1245.9	-2.2
0.4908	0.9303	1203.1	1224.9	-1.8
0.5108	0.9266	1185.2	1202.3	-1.4
0.5286	0.9232	1167.7	1180.2	-1.1
0.5453	0.9200	1149.0	1157.7	-0.8
0.5590	0.9174	1132.0	1138.0	-0.5
0.5731	0.9146	1114.2	1116.6	-0.2
0.5871	0.9117	1095.0	1094.2	0.1
0.6005	0.9090	1075.7	1071.8	0.4
0.6130	0.9064	1056.2	1049.9	0.6
0.6248	0.9039	1036.4	1028.5	0.8
0.6353	0.9016	1018.5	1008.8	1.0
0.6448	0.8996	1002.5	990.5	1.2
0.6477	0.8989	997.2	984.9	1.2
0.6542	0.8975	985.4	972.0	1.4
0.6566	0.8970	980.8	967.1	1.4
0.6633	0.8955	968.4	953.5	1.5
0.6658	0.8949	963.0	948.4	1.5
0.6723	0.8935	951.3	934.9	1.7
0.6753	0.8928	944.6	928.6	1.7
0.6849	0.8906	925.6	908.1	1.9
0.6949	0.8883	905.5	886.2	2.1
0.7051	0.8859	882.5	863.4	2.2
0.7159	0.8833	859.5	838.7	2.4
0.7268	0.8807	835.2	813.2	2.6
0.7381	0.8780	809.0	786.2	2.8
0.7497	0.8751	781.6	757.8	3.0
0.7616	0.8721	752.2	728.0	3.2
0.7739	0.8689	721.3	696.4	3.4
0.7864	0.8657	688.5	663.7	3.6
0.7995	0.8622	653.2	628.6	3.8
0.8131	0.8585	615.3	591.4	3.9
0.8272	0.8547	575.8	551.9	4.1
0.8420	0.8505	532.9	509.5	4.4
0.8572	0.8461	487.8	465.0	4.7
0.8730	0.8415	438.8	417.7	4.8
0.8895	0.8365	386.6	367.1	5.0
0.9062	0.8314	333.0	314.8	5.5
0.9236	0.8259	273.9	259.0	5.4
0.9415	0.8201	212.8	200.4	5.8
0.9603	0.8139	146.0	137.5	5.9
0.9798	0.8072	75.5	70.7	6.4

RMS DEVIATION= 3.3

TABLE A55:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-BUTANOL+N-DODECANE
DELTA H IN JOULES/MOLE

B(1)= 8.159353 B(2)= 0.005642
B(3)= 0.004932 B(4)= 0.000133

X	XCH2	Y	YPRED	DEVP
0.0447	0.9962	717.5	731.3	-1.9
0.0896	0.9921	1007.6	1064.0	-5.6
0.1668	0.9846	1247.7	1358.6	-8.9
0.2322	0.9776	1358.5	1488.5	-9.6
0.2878	0.9712	1413.3	1548.6	-9.6
0.3361	0.9652	1435.7	1572.0	-9.5
0.3786	0.9595	1443.8	1573.6	-9.0
0.4160	0.9542	1438.7	1561.4	-8.5
0.4494	0.9492	1426.5	1540.5	-8.0
0.4796	0.9445	1407.9	1513.7	-7.5
0.5064	0.9401	1386.0	1483.8	-7.1
0.5307	0.9359	1362.3	1451.9	-6.6
0.5523	0.9321	1338.2	1419.8	-6.1
0.5720	0.9285	1313.4	1387.4	-5.6
0.5905	0.9249	1286.7	1354.3	-5.3
0.6073	0.9216	1261.1	1322.1	-4.8
0.6229	0.9185	1235.1	1290.4	-4.5
0.6375	0.9154	1209.3	1259.0	-4.1
0.6510	0.9125	1183.5	1228.7	-3.8
0.6629	0.9099	1160.7	1200.8	-3.5
0.6739	0.9075	1138.6	1174.2	-3.1
0.6847	0.9050	1115.7	1147.2	-2.8
0.6948	0.9026	1093.3	1121.2	-2.5
0.6975	0.9020	1086.8	1114.1	-2.5
0.7040	0.9005	1072.6	1096.9	-2.3
0.7058	0.9000	1067.9	1092.0	-2.3
0.7125	0.8984	1052.5	1073.9	-2.0
0.7142	0.8980	1047.3	1069.2	-2.1
0.7202	0.8965	1034.0	1052.6	-1.8
0.7228	0.8959	1026.8	1045.3	-1.8
0.7316	0.8936	1004.4	1020.3	-1.6
0.7406	0.8913	980.9	994.2	-1.4
0.7595	0.8864	930.3	937.4	-0.8
0.7694	0.8837	902.7	906.7	-0.4
0.7793	0.8809	872.5	875.3	-0.3
0.7895	0.8780	843.9	842.3	0.2
0.8002	0.8749	811.6	806.8	0.6
0.8111	0.8717	776.7	769.9	0.9
0.8221	0.8684	742.1	731.8	1.4
0.8338	0.8647	703.3	690.3	1.8
0.8459	0.8608	661.5	646.4	2.3
0.8582	0.8568	618.4	600.8	2.9
0.8708	0.8525	571.8	553.0	3.3
0.8837	0.8480	522.7	502.9	3.8
0.8966	0.8434	472.3	451.6	4.4
0.9100	0.8384	417.9	397.2	5.0
0.9242	0.8329	358.3	338.2	5.6
0.9387	0.8271	295.5	276.5	6.4
0.9534	0.8210	228.9	212.5	7.1
0.9683	0.8146	158.3	146.2	7.6
0.9841	0.8075	80.5	74.2	7.9

RMS DEVIATION= 5.1

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TABLE A56:

 HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-PENTANOL+N-OCTANE
DELTA H IN JOULES/MOLE
   B(1)=  8.159353     B(2)=  0.005642
  B(3)=  0.004932      B(4)=  0.000133
   X           XCH2        Y            YPRED       DEVP

  0.0277      0.9965      464.7        458.5         1.3
  0.0567      0.9928      684.8        683.9         0.1
  0.1087      0.9860      877.1        898.9        -2.5
  0.1560      0.9797      974.4       1009.0        -3.6
  0.1994      0.9738     1032.2       1072.7        -3.9
  0.2377      0.9684     1067.4       1108.2        -3.8
  0.2729      0.9634     1089.6       1127.2        -3.5
  0.3054      0.9587     1101.0       1134.9        -3.1
  0.3350      0.9543     1105.9       1134.6        -2.6
  0.3623      0.9502     1106.2       1128.7        -2.0
  0.3874      0.9464     1102.1       1118.9        -1.5
  0.4105      0.9428     1095.2       1106.3        -1.0
  0.4315      0.9395     1086.7       1092.2        -0.5
  0.4510      0.9365     1075.8       1076.8        -0.1
  0.4688      0.9336     1064.6       1060.9         0.3
  0.4863      0.9308     1052.0       1043.6         0.8
  0.5024      0.9282     1038.5       1026.4         1.2
  0.5170      0.9258     1025.1       1009.7         1.5
  0.5304      0.9236     1011.2        993.4         1.8
  0.5427      0.9215      998.2        977.8         2.0
  0.5552      0.9194      984.4        961.1         2.4
  0.5673      0.9174      970.1        944.4         2.7
  0.5732      0.9164      951.9        936.0         1.7
  0.5810      0.9150      951.4        924.6         2.8
  0.5826      0.9148      939.4        922.2         1.8
  0.5910      0.9133      938.4        909.7         3.1
  0.5927      0.9130      925.8        907.1         2.0
  0.6012      0.9116      924.0        894.0         3.2
  0.6032      0.9112      910.7        890.9         2.2
  0.6106      0.9099      910.6        879.2         3.5
  0.6139      0.9094      894.8        873.9         2.3
  0.6198      0.9083      896.9        864.3         3.6
  0.6248      0.9074      878.9        856.1         2.6
  0.6286      0.9068      883.4        849.8         3.8
  0.6364      0.9054      860.6        836.7         2.8
  0.6483      0.9033      840.9        816.2         2.9
  0.6605      0.9011      820.3        794.6         3.1
  0.6734      0.8988      797.0        771.2         3.2
  0.6867      0.8964      773.0        746.4         3.4
  0.7005      0.8938      746.9        720.0         3.6
  0.7150      0.8912      718.1        691.5         3.7
  0.7299      0.8884      688.6        661.5         3.9
  0.7453      0.8855      655.7        629.6         4.0
  0.7617      0.8824      621.0        594.9         4.2
  0.7784      0.8792      583.4        558.6         4.3
  0.7960      0.8758      541.9        519.3         4.2
  0.8146      0.8721      499.3        476.8         4.5
  0.8344      0.8682      450.6        430.5         4.5
  0.8549      0.8641      398.9        381.2         4.4
  0.8766      0.8597      343.2        327.8         4.5
  0.8988      0.8551      283.7        271.8         4.2
  0.9228      0.8501      219.1        209.7         4.3
  0.9473      0.8448      150.7        144.8         3.9
  0.9737      0.8391       76.1         73.1         3.9
                                          RMS DEVIATION=         3.1
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TABLE A57:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-PENTANOL+N-NONANE
DELTA H IN JOULES/MOLE

B(1)= 8.159353 B(2)= 0.005642
B(3)= 0.004932 B(4)= 0.000133

X	XCH2	Y	YPRED	DEVP
0.0302	0.9966	506.2	505.0	0.2
0.0611	0.9931	738.1	750.8	-1.7
0.1167	0.9865	944.1	986.1	-4.4
0.1658	0.9805	1044.9	1102.2	-5.5
0.2104	0.9749	1104.6	1168.1	-5.7
0.2510	0.9696	1141.7	1205.2	-5.6
0.2875	0.9647	1162.3	1223.6	-5.3
0.3207	0.9601	1174.0	1229.8	-4.8
0.3509	0.9558	1177.6	1227.6	-4.3
0.3778	0.9520	1220.0	1219.9	0.0
0.4029	0.9483	1209.1	1208.2	0.1
0.4259	0.9448	1228.4	1193.8	2.8
0.4473	0.9416	1211.9	1177.4	2.8
0.4666	0.9386	1194.6	1160.2	2.9
0.4845	0.9358	1176.9	1142.3	2.9
0.5014	0.9331	1158.5	1123.8	3.0
0.5173	0.9305	1140.1	1104.9	3.1
0.5322	0.9281	1122.6	1086.0	3.3
0.5462	0.9258	1105.0	1067.1	3.4
0.5601	0.9235	1086.1	1047.4	3.6
0.5730	0.9213	1067.5	1028.2	3.7
0.5855	0.9192	1048.7	1008.8	3.8
0.5964	0.9173	1031.9	99[illegible]3	3.9
0.6069	0.9155	1015.1	973.9	4.1
0.6109	0.9148	993.6	967.2	2.7
0.6168	0.9137	998.6	957.0	4.2
0.6205	0.9131	978.2	950.6	2.8
0.6250	0.9123	985.1	942.7	4.3
0.6303	0.9113	962.6	933.3	3.0
0.6337	0.9107	970.0	927.2	4.4
0.6401	0.9096	945.9	916.5	3.2
0.6503	0.9077	927.8	896.5	3.4
0.6612	0.9058	908.6	875.8	3.6
0.6719	0.9038	889.3	854.9	3.9
0.6830	0.9017	866.7	832.7	3.9
0.6949	0.8995	844.0	808.3	4.2
0.7068	0.8973	819.6	783.3	4.4
0.7187	0.8950	794.1	757.7	4.6
0.7317	0.8925	766.0	729.1	4.8
0.7451	0.8899	736.2	698.9	5.1
0.7589	0.8871	703.9	667.0	5.2
0.7732	0.8843	668.8	633.2	5.3
0.7882	0.8812	632.2	596.9	5.6
0.8037	0.8780	592.3	558.6	5.7
0.8194	0.8747	551.7	518.8	6.0
0.8363	0.8712	505.7	474.9	6.1
0.8539	0.8674	457.2	428.2	6.4
0.8722	0.8634	404.1	378.4	6.3
0.8911	0.8592	348.2	325.8	6.4
0.9109	0.8547	287.7	269.4	6.4
0.9316	0.8499	222.3	209.1	6.0
0.9532	0.8448	153.5	144.6	5.8
0.9760	0.8393	79.0	75.0	5.1

RMS DEVIATION= 4.4

TABLE A58:

```
 HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-PENTANOL+N-DODECANE
DELTA H IN JOULES/MOLE
    B(1)=  8.159353     B(2)=  0.005642
   B(3)=  0.004932      B(4)=  0.000133
    X          XCH2         Y            YPRED       DEVP

  0.0399     0.9966       641.9        667.0      -3.9
  0.0762     0.9934       908.2        959.2      -5.6
  0.1440     0.9871      1149.2       1249.0      -8.7
  0.2032     0.9812      1260.8       1382.4      -9.6
  0.2560     0.9755      1321.6       1450.0      -9.7
  0.3014     0.9704      1353.5       1480.0      -9.4
  0.3419     0.9656      1367.4       1488.8      -8.9
  0.3772     0.9613      1371.0       1484.3      -8.3
  0.4101     0.9570      1365.4       1470.5      -7.7
  0.4398     0.9530      1355.3       1450.8      -7.0
  0.4657     0.9494      1343.9       1428.1      -6.3
  0.4893     0.9460      1327.9       1403.2      -5.7
  0.5100     0.9430      1311.0       1378.1      -5.1
  0.5276     0.9403      1295.8       1354.3      -4.5
  0.5454     0.9375      1277.4       1328.2      -4.0
  0.5614     0.9350      1260.5       1302.9      -3.4
  0.5774     0.9324      1240.8       1275.9      -2.8
  0.5924     0.9299      1220.3       1249.0      -2.4
  0.6071     0.9274      1199.1       1221.3      -1.9
  0.6197     0.9252      1148.7       1196.4      -4.2
  0.6316     0.9231      1131.8       1172.0      -3.6
  0.6434     0.9210      1143.1       1146.9      -0.3
  0.6544     0.9189      1123.8       1122.8       0.1
  0.6641     0.9171      1090.6       1100.8      -0.9
  0.6648     0.9170      1104.4       1099.2       0.5
  0.6730     0.9155      1072.6       1080.2      -0.7
  0.6743     0.9152      1086.2       1077.1       0.8
  0.6817     0.9138      1055.6       1059.5      -0.4
  0.6833     0.9135      1068.4       1055.7       1.2
  0.6907     0.9121      1035.9       1037.7      -0.2
  0.6918     0.9119      1050.9       1035.0       1.5
  0.6983     0.9106      1037.0       1018.8       1.7
  0.7000     0.9103      1016.4       1014.6       0.2
  0.7096     0.9083       994.9        990.2       0.5
  0.7193     0.9064       972.0        964.9       0.7
  0.7298     0.9042       947.1        937.0       1.1
  0.7404     0.9020       921.3        908.1       1.4
  0.7510     0.8998       894.4        878.6       1.8
  0.7618     0.8975       865.6        847.8       2.0
  0.7732     0.8950       833.5        814.6       2.3
  0.7852     0.8923       800.5        778.8       2.7
  0.7972     0.8895       765.7        742.2       3.1
  0.8098     0.8866       728.4        702.8       3.5
  0.8227     0.8835       687.8        661.5       3.8
  0.8358     0.8803       646.4        618.7       4.3
  0.8495     0.8769       601.0        572.8       4.7
  0.8641     0.8732       550.6        522.7       5.1
  0.8791     0.8693       497.8        470.0       5.6
  0.8944     0.8652       441.6        415.0       6.0
  0.9102     0.8608       380.4        356.8       6.2
  0.9270     0.8560       314.9        293.4       6.8
  0.9445     0.8509       243.3        225.7       7.2
  0.9627     0.8453       166.6        153.5       7.9
  0.9811     0.8395        85.1         78.7       7.4
---------------------------------------------------------------------
                                         RMS DEVIATION=          4.9
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TABLE A59:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-HEXANOL+N-OCTANE
DELTA H IN JOULES/MOLE

B(1)= 8.159353 B(2)= 0.005642
B(3)= 0.004932 B(4)= 0.000133

X	XCH2	Y	YPRED	DEVP
0.0243	0.9970	410.7	413.6	-0.7
0.0491	0.9938	620.8	622.1	-0.2
0.0954	0.9879	807.1	830.9	-3.0
0.1379	0.9825	899.7	938.5	-4.3
0.1773	0.9773	955.7	1001.9	-4.8
0.2122	0.9728	988.7	1038.6	-5.1
0.2435	0.9686	1008.9	1059.6	-5.0
0.2732	0.9646	1022.0	1070.7	-4.8
0.3010	0.9609	1028.6	1074.5	-4.5
0.3268	0.9574	1030.5	1072.8	-4.1
0.3499	0.9543	1029.5	1067.4	-3.7
0.3719	0.9512	1025.9	1059.1	-3.2
0.3933	0.9483	1019.8	1048.2	-2.8
0.4127	0.9456	1012.4	1036.2	-2.3
0.4310	0.9431	1003.5	1023.0	-1.9
0.4478	0.9407	994.3	1009.3	-1.5
0.4634	0.9385	984.2	995.4	-1.1
0.4781	0.9364	974.4	981.3	-0.7
0.4931	0.9343	962.1	965.8	-0.4
0.5061	0.9325	950.9	951.6	-0.1
0.5181	0.9308	939.8	937.8	0.2
0.5287	0.9292	930.2	925.2	0.5
0.5401	0.9276	919.3	911.1	0.9
0.5474	0.9265	899.8	901.7	-0.2
0.5514	0.9260	906.8	896.5	1.1
0.5570	0.9252	889.8	889.1	0.1
0.5617	0.9245	895.2	882.9	1.4
0.5670	0.9237	878.4	875.7	0.3
0.5718	0.9230	883.2	869.0	1.6
0.5775	0.9222	865.9	861.1	0.6
0.5809	0.9217	872.1	856.3	1.8
0.5883	0.9206	852.3	845.7	0.8
0.5997	0.9190	836.8	828.9	0.9
0.6114	0.9173	820.9	811.2	1.2
0.6237	0.9154	803.4	792.2	1.4
0.6366	0.9135	784.2	771.6	1.6
0.6501	0.9115	763.4	749.4	1.8
0.6640	0.9095	742.3	726.0	2.2
0.6783	0.9074	718.3	701.3	2.4
0.6932	0.9051	692.7	674.8	2.6
0.7086	0.9028	664.9	646.7	2.7
0.7249	0.9004	635.2	616.3	3.0
0.7416	0.8978	603.1	584.3	3.1
0.7592	0.8951	568.6	549.7	3.3
0.7786	0.8922	527.8	510.6	3.3
0.7986	0.8891	485.6	469.2	3.4
0.8196	0.8859	439.9	424.6	3.5
0.8411	0.8825	392.1	377.9	3.6
0.8638	0.8790	339.5	327.3	3.6
0.8887	0.8750	280.5	270.5	3.6
0.9143	0.8710	217.6	210.6	3.2
0.9413	0.8666	150.3	145.9	3.0
0.9696	0.8621	77.9	76.4	2.0

RMS DEVIATION= 2.7

```
HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-OCTANOL+N-HEPTANE
DELTA H IN JOULES/MOLE
   B(1)=  8.159353      B(2)=  0.005642
  B(3)=  0.004932       B(4)=  0.000133
   X           XCH2          Y          YPRED        DEVP

  0.0170      0.9976       289.7       301.7        -4.2
  0.0336      0.9952       417.0       461.1       -10.6
  0.0657      0.9908       635.3       634.3         0.2
  0.0971      0.9865       720.7       731.2        -1.5
  0.1276      0.9824       774.6       792.4        -2.3
  0.1562      0.9786       808.2       831.6        -2.9
  0.1825      0.9752       829.1       856.7        -3.3
  0.2079      0.9720       842.3       873.2        -3.7
  0.2302      0.9691       851.7       882.4        -3.6
  0.2514      0.9665       855.4       887.2        -3.7
  0.2704      0.9642       858.6       888.7        -3.5
  0.2897      0.9618       858.9       887.7        -3.4
  0.3078      0.9596       858.2       884.7        -3.1
  0.3263      0.9574       855.8       879.7        -2.8
  0.3433      0.9553       851.5       873.5        -2.6
  0.3591      0.9535       847.2       866.5        -2.3
  0.3735      0.9518       842.2       859.1        -2.0
  0.3875      0.9502       836.4       851.0        -1.7
  0.4001      0.9487       830.7       843.0        -1.5
  0.4120      0.9473       825.1       834.9        -1.2
  0.4237      0.9460       819.5       826.3        -0.8
  0.4354      0.9447       813.2       817.3        -0.5
  0.4472      0.9434       806.4       807.7        -0.2
  0.4580      0.9421       800.1       798.5         0.2
  0.4613      0.9418       791.7       795.6        -0.5
  0.4695      0.9409       792.5       788.2         0.5
  0.4712      0.9407       784.1       786.7        -0.3
  0.4817      0.9395       777.7       776.9         0.1
  0.4819      0.9395       782.7       776.7         0.8
  0.4918      0.9384       776.0       767.2         1.1
  0.4922      0.9384       768.1       766.8         0.2
  0.5016      0.9373       768.2       757.4         1.4
  0.5036      0.9371       757.5       755.4         0.3
  0.5103      0.9364       760.7       748.5         1.6
  0.5153      0.9358       747.0       743.3         0.5
  0.5178      0.9356       754.3       740.7         1.8
  0.5256      0.9347       747.8       732.4         2.1
  0.5275      0.9345       735.8       730.3         0.7
  0.5402      0.9331       723.3       716.3         1.0
  0.5535      0.9317       709.8       701.2         1.2
  0.5675      0.9302       695.3       684.8         1.5
  0.5821      0.9287       678.7       667.2         1.7
  0.5975      0.9271       661.4       648.1         2.0
  0.6137      0.9254       642.0       627.4         2.3
  0.6308      0.9236       619.5       604.9         2.3
  0.6488      0.9218       596.8       580.6         2.7
  0.6680      0.9199       571.7       553.9         3.1
  0.6885      0.9178       542.8       524.6         3.4
  0.7111      0.9156       509.7       491.4         3.6
  0.7348      0.9132       474.1       455.6         3.9
  0.7598      0.9108       434.4       416.9         4.0
  0.7868      0.9082       389.8       373.9         4.1
  0.8146      0.9056       343.6       328.5         4.4
  0.8462      0.9027       287.2       275.5         4.1
  0.8797      0.8996       226.8       217.9         3.9
  0.9165      0.8962       157.5       153.0         2.9
  0.9573      0.8926        81.1        79.2         2.4
                                    RMS DEVIATION=        2.8
```

TABLE A61:

HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-OCTANOL+N-OCTANE
DELTA H IN JOULES/MOLE

B(1)= 8.159353 B(2)= 0.005642
B(3)= 0.004932 B(4)= 0.000133

X	XCH2	Y	YPRED	DEVP
0.0189	0.9976	330.5	338.0	-2.3
0.0348	0.9957	494.9	497.8	-0.6
0.0693	0.9914	676.8	697.8	-3.1
0.1020	0.9874	771.1	805.7	-4.5
0.1324	0.9837	827.4	871.4	-5.3
0.1607	0.9803	863.3	913.8	-5.8
0.1887	0.9770	888.5	943.0	-6.1
0.2149	0.9738	903.8	961.5	-6.4
0.2384	0.9711	914.9	971.9	-6.2
0.2580	0.9688	918.9	976.9	-6.3
0.2750	0.9668	922.7	978.7	-6.1
0.2920	0.9648	924.1	978.4	-5.9
0.3104	0.9626	923.4	975.9	-5.7
0.3279	0.9606	921.9	971.5	-5.4
0.3456	0.9586	918.4	965.2	-5.1
0.3613	0.9568	914.7	958.2	-4.8
0.3766	0.9550	910.4	950.2	-4.4
0.3918	0.9533	904.6	941.0	-4.0
0.4059	0.9517	898.3	931.6	-3.7
0.4192	0.9502	891.6	921.8	-3.4
0.4323	0.9487	884.5	911.5	-3.1
0.4453	0.9473	876.4	900.5	-2.8
0.4568	0.9460	868.2	890.3	-2.5
0.4679	0.9447	860.2	879.9	-2.3
0.4785	0.9436	852.4	869.5	-2.0
0.4838	0.9430	845.6	864.2	-2.2
0.4878	0.9425	846.2	860.1	-1.6
0.4935	0.9419	838.6	854.2	-1.9
0.4984	0.9414	838.2	849.0	-1.3
0.5034	0.9408	830.0	843.6	-1.6
0.5084	0.9402	830.5	838.1	-0.9
0.5141	0.9396	821.1	831.8	-1.3
0.5183	0.9392	822.4	827.1	-0.6
0.5253	0.9384	810.4	819.0	-1.1
0.5293	0.9379	811.7	814.4	-0.3
0.5367	0.9371	798.9	805.6	-0.8
0.5489	0.9358	786.9	790.8	-0.5
0.5614	0.9344	773.9	775.1	-0.2
0.5747	0.9330	759.2	758.0	0.2
0.5884	0.9315	743.0	739.7	0.4
0.6031	0.9299	725.5	719.6	0.8
0.6183	0.9283	705.9	698.2	1.1
0.6346	0.9265	684.3	674.5	1.4
0.6517	0.9247	660.5	648.9	1.8
0.6696	0.9228	634.7	621.4	2.1
0.6884	0.9208	606.6	591.6	2.5
0.7088	0.9186	575.2	558.5	2.9
0.7311	0.9163	539.5	521.2	3.4
0.7780	0.9114	457.2	439.3	3.9
0.8035	0.9087	409.9	393.0	4.1
0.8306	0.9059	358.5	342.5	4.5
0.8596	0.9030	300.8	287.1	4.5
0.8909	0.8998	237.2	225.7	4.8
0.9249	0.8964	165.8	157.2	5.2
0.9608	0.8928	87.1	83.0	4.6

RMS DEVIATION= 3.6

```
 HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-OCTANOL+N-NONANE
DELTA H IN JOULES/MOLE
     B(1)=   8.159353       B(2)=   0.005642
    B(3)=   0.004932        B(4)=   0.000133
     X           XCH2        Y               YPRED      DEVP

    0.0223      0.9975      334.5       392.7      -17.4
    0.0431      0.9952      542.6       589.5       -8.6
    0.0844      0.9906      744.8       806.1       -8.2
    0.1223      0.9864      839.5       916.6       -9.2
    0.1580      0.9824      895.9       982.5       -9.7
    0.1904      0.9788      930.6      1021.8       -9.8
    0.2213      0.9754      953.3      1045.9       -9.7
    0.2496      0.9723      967.8      1058.8       -9.4
    0.2743      0.9695      974.6      1064.1       -9.2
    0.2959      0.9671      976.7      1064.7       -9.0
    0.3175      0.9647      977.9      1061.8       -8.6
    0.3384      0.9624      977.9      1056.1       -8.0
    0.3582      0.9602      976.8      1048.2       -7.3
    0.3770      0.9581      972.1      1038.5       -6.8
    0.3949      0.9561      966.3      1027.5       -6.3
    0.4113      0.9543      960.3      1016.0       -5.8
    0.4268      0.9526      953.1      1003.9       -5.3
    0.4296      0.9523      965.2      1001.6       -3.8
    0.4434      0.9507      957.3       989.7       -3.4
    0.4573      0.9492      920.2       976.8       -6.2
    0.4705      0.9477      939.7       963.8       -2.6
    0.4828      0.9464      930.6       951.1       -2.2
    0.4947      0.9450      921.1       938.1       -1.8
    0.5058      0.9438      912.4       925.5       -1.4
    0.5115      0.9432      900.3       918.8       -2.1
    0.5165      0.9426      904.0       912.9       -1.0
    0.5213      0.9421      890.4       907.1       -1.9
    0.5276      0.9414      894.5       899.4       -0.5
    0.5315      0.9409      880.0       894.5       -1.6
    0.5376      0.9403      885.7       886.8       -0.1
    0.5420      0.9398      870.1       881.1       -1.3
    0.5476      0.9392      876.0       873.8        0.2
    0.5529      0.9386      858.3       866.8       -1.0
    0.5577      0.9380      865.1       860.4        0.5
    0.5646      0.9373      844.9       851.0       -0.7
    0.5658      0.9371      856.4       849.4        0.8
    0.5763      0.9360      831.2       834.7       -0.4
    0.5886      0.9346      816.3       817.1       -0.1
    0.6021      0.9331      798.7       797.2        0.2
    0.6154      0.9316      780.1       777.0        0.4
    0.6292      0.9301      761.5       755.5        0.8
    0.6444      0.9284      739.9       731.2        1.2
    0.6606      0.9266      715.7       704.5        1.6
    0.6770      0.9248      690.1       676.6        2.0
    0.6942      0.9229      662.3       646.7        2.4
    0.7129      0.9208      630.4       613.2        2.7
    0.7321      0.9187      596.6       577.9        3.1
    0.7521      0.9164      559.3       540.1        3.4
    0.7731      0.9141      519.1       499.4        3.8
    0.7954      0.9116      474.1       455.0        4.0
    0.8198      0.9089      423.8       405.2        4.4
    0.8452      0.9061      369.4       352.0        4.7
    0.8727      0.9030      307.7       292.8        4.9
    0.9017      0.8998      240.0       228.7        4.7
    0.9330      0.8963      166.2       157.8        5.0
    0.9653      0.8927       87.2        82.7        5.2
                                              RMS DEVIATION=        5.5
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```
 HEATS OF MIXING AT 55 DEG.C FOR THE SYSTEM N-OCTANOL+N-DODECANE
DELTA H IN JOULES/MOLE
   B(1)=  8.159353     B(2)=  0.005642
  B(3)=  0.004932      B(4)=  0.000133
   X         XCH2      Y           YPRED      DEVP

  0.0271    0.9977     473.1      489.9       -3.5
  0.0547    0.9954     732.9      760.4       -3.7
  0.1037    0.9911     952.7     1024.2       -7.5
  0.1481    0.9872    1057.7     1155.8       -9.3
  0.1885    0.9835    1117.0     1229.1      -10.0
  0.2258    0.9801    1149.8     1271.1      -10.6
  0.2597    0.9769    1167.0     1293.1      -10.8
  0.2912    0.9738    1176.5     1302.3      -10.7
  0.3190    0.9711    1177.4     1302.7      -10.6
  0.3449    0.9685    1175.6     1297.3      -10.4
  0.3698    0.9660    1169.0     1287.3      -10.1
  0.3928    0.9637    1160.3     1274.1       -9.8
  0.4142    0.9615    1150.8     1258.8       -9.4
  0.4341    0.9594    1140.1     1241.9       -8.9
  0.4523    0.9575    1129.1     1224.4       -8.4
  0.4699    0.9556    1116.2     1205.6       -8.0
  0.4865    0.9538    1101.7     1186.3       -7.7
  0.5013    0.9522    1087.2     1167.9       -7.4
  0.5149    0.9508    1073.8     1149.9       -7.1
  0.5279    0.9493    1060.9     1131.9       -6.7
  0.5402    0.9480    1048.7     1114.0       -6.2
  0.5523    0.9466    1035.8     1095.7       -5.8
  0.5645    0.9452    1021.5     1076.5       -5.4
  0.5760    0.9439    1001.1     1057.8       -5.7
  0.5761    0.9439    1007.1     1057.6       -5.0
  0.5851    0.9429     989.5     1042.5       -5.4
  0.5864    0.9427     993.9     1040.3       -4.7
  0.5947    0.9418     976.7     1026.0       -5.1
  0.5967    0.9416     979.4     1022.5       -4.4
  0.6047    0.9406     962.8     1008.4       -4.7
  0.6058    0.9405     966.7     1006.4       -4.1
  0.6145    0.9395     954.4      990.7       -3.8
  0.6156    0.9394     947.7      988.6       -4.3
  0.6265    0.9381     930.8      968.4       -4.0
  0.6379    0.9368     912.6      946.6       -3.7
  0.6498    0.9353     894.1      923.3       -3.3
  0.6620    0.9339     873.1      898.8       -2.9
  0.6748    0.9324     851.7      872.4       -2.4
  0.6879    0.9308     827.9      844.7       -2.0
  0.7014    0.9291     802.1      815.5       -1.7
  0.7150    0.9274     775.2      785.3       -1.3
  0.7298    0.9256     745.8      751.6       -0.8
  0.7449    0.9237     713.9      716.3       -0.3
  0.7615    0.9216     677.3      676.5        0.1
  0.7793    0.9193     637.6      632.8        0.8
  0.7973    0.9170     594.6      587.3        1.2
  0.8157    0.9146     548.6      539.7        1.6
  0.8353    0.9120     499.0      487.6        2.3
  0.8552    0.9094     445.7      433.4        2.8
  0.8772    0.9064     383.3      371.9        3.0
  0.8994    0.9033     319.9      308.2        3.7
  0.9227    0.9001     249.1      239.6        3.8
  0.9470    0.8966     174.8      166.3        4.9
  0.9724    0.8929      91.1       87.6        3.7
                                         RMS DEVIATION=        6.1
```

TABLE A64:

```
HEATS OF MIXING OF SYSTEM ETHANOL HEXANE AT 30 DEG.C,
X=MOL.FRACT. OF ALCOHOL, DATA OF VAN NESS
    B(1)=  8.029668      B(2)=  0.004725
   B(3)=  0.002373      B(4)=  0.000075
    X          XCH2         Y            YPRED      DEVP

   0.0100     0.9983      178.3        168.9         5.3
   0.0200     0.9966      256.0        253.1         1.1
   0.0300     0.9949      303.2        309.2        -2.0
   0.0400     0.9932      339.1        352.3        -3.9
   0.0500     0.9915      368.6        388.0        -5.3
   0.0750     0.9870      426.7        459.2        -7.6
   0.1000     0.9825      469.8        515.7        -9.8
   0.1250     0.9778      505.3        562.8       -11.4
   0.1500     0.9730      534.2        602.8       -12.8
   0.1750     0.9680      557.3        636.8       -14.3
   0.2000     0.9630      577.6        665.5       -15.2
   0.3000     0.9412      621.6        735.7       -18.4
   0.4000     0.9167      628.8        746.6       -18.7
   0.5000     0.8889      602.5        708.5       -17.6
   0.6000     0.8571      554.4        629.1       -13.5
   0.7000     0.8205      476.7        514.1        -7.9
   0.8000     0.7778      368.0        368.5        -0.1
   0.9000     0.7273      218.7        196.0        10.4
                                        RMS DEVIATION=       11.3
```

TABLE A65:

```
HEATS OF MIXING AT 30 DEG FOR SYSTEM ETHANOL NONANE
X=MOL.FRACT. OF ALCOHOL, DATA OF VAN NESS
    B(1)=  0.029668     B(2)=  0.004725
   B(3)=  0.002373      B(4)=  0.000075
    X          XCH2        Y          YPRED      DEVP

   0.0100     0.9989      193.7      191.7        1.1
   0.0200     0.9977      291.3      302.0       -3.7
   0.0300     0.9966      349.5      377.8       -8.1
   0.0400     0.9954      394.0      435.6      -10.6
   0.0500     0.9943      430.8      482.5      -12.0
   0.0750     0.9912      498.1      573.5      -15.1
   0.1000     0.9881      543.6      643.4      -18.4
   0.1250     0.9848      583.0      701.0      -20.2
   0.1500     0.9815      617.1      750.0      -21.5
   0.1750     0.9780      646.8      792.3      -22.5
   0.2000     0.9744      670.4      828.8      -23.6
   0.3000     0.9583      730.8      927.4      -26.9
   0.4000     0.9394      746.4      960.1      -28.6
   0.5000     0.9167      730.0      933.2      -27.8
   0.6000     0.8889      684.0      850.2      -24.3
   0.7000     0.8542      606.9      713.5      -17.6
   0.8000     0.8095      491.2      525.0       -6.9
   0.9000     0.7500      311.4      286.6        8.0
                                        RMS DEVIATION=        18.5
```

TABLE A66;

```
HEATS OF MIXING AT 30 DEG. C FOR SYSTEM PROPANOL HEPTANE
X=MOL.FRACT. OF ALCOHOL, DATA OF VAN NESS
    B(1)=   8.029668      B(2)=   0.004725
   B(3)=   0.002373      B(4)=   0.000075
    X            XCH2         Y             YPRED        DEVP

  0.0100      0.9986       188.6       174.7          7.3
  0.0200      0.9971       281.5       265.5          5.7
  0.0300      0.9957       337.9       325.6          3.6
  0.0400      0.9942       378.2       370.9          1.9
  0.0500      0.9927       411.3       407.7          0.9
  0.0750      0.9889       478.7       479.0         -0.1
  0.1000      0.9851       529.2       533.8         -0.9
  0.1250      0.9811       569.8       578.5         -1.5
  0.1500      0.9771       603.1       616.0         -2.1
  0.1750      0.9730       630.9       647.5         -2.6
  0.2000      0.9688       654.4       673.9         -3.0
  0.3000      0.9508       707.7       737.1         -4.2
  0.4000      0.9310       708.0       744.1         -5.1
  0.5000      0.9091       667.5       704.5         -5.5
  0.6000      0.8846       590.4       625.0         -5.9
  0.7000      0.8571       485.1       511.0         -5.3
  0.8000      0.8261       353.6       366.5         -3.6
  0.9000      0.7907       194.4       195.2         -0.4
                                          RMS DEVIATION=        3.9
```

TABLE A67:

```
HEATS OF MIXING OF SYSTEM BUTANOL HEPTANE AT 30 DEG.C
X=MOL.FRACT. OF ALCOHOL, DATA OF VAN NESS
     B(1)=  8.029668      B(2)=  0.004725
     B(3)=  0.002373      B(4)=  0.000075
      X           XCH2        Y          YPRED      DEVP

    0.0100       0.9986     182.1       172.1        5.5
    0.0200       0.9971     273.6       260.4        4.8
    0.0300       0.9957     331.2       318.1        3.9
    0.0400       0.9942     373.2       361.1        3.3
    0.0500       0.9928     406.6       395.6        2.7
    0.0750       0.9891     467.6       461.6        1.3
    0.1000       0.9853     514.8       511.1        0.7
    0.1250       0.9815     552.3       550.9        0.3
    0.1500       0.9776     583.9       583.5        0.1
    0.1750       0.9737     610.7       610.5        0.0
    0.2000       0.9697     632.0       632.6       -0.1
    0.3000       0.9531     686.7       681.6        0.7
    0.4000       0.9355     686.4       679.6        1.0
    0.5000       0.9167     642.5       636.6        0.9
    0.6000       0.8966     559.2       559.7       -0.1
    0.7000       0.8750     447.3       453.8       -1.4
    0.8000       0.8519     313.6       323.1       -3.0
    0.9000       0.8269     162.9       170.9       -4.9
                                       RMS DEVIATION=        2.7
```

TABLE A68:

```
HEATS OF MIXING OF SYSTEM PENTANOL HEXANE AT 30 DEG.C
X=MOL.FRACT. OF ALCOHOL, DATA OF VAN NESS
    B(1)=  0.029668     B(2)=  0.004725
   B(3)=  0.002373      B(4)=  0.000075
    X           XCH2        Y            YPRED      DEVP

   0.0100     0.9983      177.1        160.9         9.2
   0.0200     0.9967      257.0        237.6         7.5
   0.0300     0.9950      304.1        286.7         5.7
   0.0400     0.9933      338.7        322.8         4.7
   0.0500     0.9917      365.7        351.8         3.8
   0.0750     0.9875      417.6        406.8         2.6
   0.1000     0.9833      456.3        447.7         1.9
   0.1250     0.9792      486.7        479.9         1.4
   0.1500     0.9750      512.5        505.7         1.3
   0.1750     0.9708      532.7        526.4         1.2
   0.2000     0.9667      550.4        542.8         1.4
   0.3000     0.9500      590.1        573.3         2.9
   0.4000     0.9333      585.6        560.8         4.2
   0.5000     0.9167      540.0        516.2         4.4
   0.6000     0.9000      458.4        446.5         2.6
   0.7000     0.8833      357.0        356.7         0.1
   0.8000     0.8667      243.2        250.6        -3.0
   0.9000     0.8500      122.4        130.9        -7.0
                                         RMS DEVIATION=        4.3
```

TABLE A69:

```
HEATS OF MIXING AT 30 DEG. C FOR SYSTEM OCTANOL+HEPTANE
X=MOL.FRACT. OF ALCOHOL, DATA OF VAN NESS
    B(1)=  8.029668      B(2)=  0.004725
    B(3)=  0.002373      B(4)=  0.000075
     X          XCH2          Y           YPRED      DEVP

    0.0100     0.9986       176.5        164.2        7.0
    0.0200     0.9972       259.3        245.3        5.4
    0.0300     0.9958       306.4        296.3        3.3
    0.0400     0.9944       337.9        332.9        1.5
    0.0500     0.9930       362.4        361.2        0.3
    0.0750     0.9895       409.3        412.2       -0.7
    0.1000     0.9861       442.8        447.6       -1.1
    0.1250     0.9828       468.1        474.0       -1.3
    0.1500     0.9795       487.0        494.0       -1.4
    0.1750     0.9762       501.0        509.2       -1.6
    0.2000     0.9730       512.0        520.3       -1.6
    0.3000     0.9605       537.6        534.4        0.6
    0.4000     0.9487       530.4        512.6        3.4
    0.5000     0.9375       495.0        464.9        6.1
    0.6000     0.9268       432.0        397.5        8.0
    0.7000     0.9167       342.3        314.6        8.1
    0.8000     0.9070       236.8        219.3        7.4
    0.9000     0.8977       118.8        113.9        4.2
                                        RMS DEVIATION=        4.4
```

TABLE A70:

```
HEATS OF MIXING OF OCTANOL+NONANE AT 30 DEG. C
X=MOL.FRACT. OF ALCOHOL, DATA OF VAN NESS
    B(1)=   8.029668      B(2)=   0.004725
   B(3)=  0.002373        B(4)=   0.000075
    X          XCH2         Y            YPRED        DEVP

   0.0100     0.9989      184.2         177.9          3.5
   0.0200     0.9978      281.5         275.3          2.2
   0.0300     0.9967      338.4         338.9         -0.1
   0.0400     0.9956      379.8         384.9         -1.4
   0.0500     0.9944      410.9         420.5         -2.3
   0.0750     0.9917      466.9         484.0         -3.7
   0.1000     0.9889      505.8         527.4         -4.3
   0.1250     0.9861      535.9         559.5         -4.4
   0.1500     0.9833      558.4         584.1         -4.6
   0.1750     0.9806      577.5         602.9         -4.4
   0.2000     0.9778      592.0         617.1         -4.2
   0.3000     0.9667      623.7         639.3         -2.5
   0.4000     0.9556      621.6         619.7          0.3
   0.5000     0.9444      587.5         568.4          3.3
   0.6000     0.9333      511.2         491.4          3.9
   0.7000     0.9222      413.7         393.2          5.0
   0.8000     0.9111      291.2         276.9          4.9
   0.9000     0.9000      150.3         145.1          3.5
                                             RMS DEVIATION=         3.5
```

TABLE A71:

```
HEATS OF MIXING OF ETHANOL+HEXANE AT 45 DEG. C
X=MOL.FRACT. OF ALCOHOL, DATA OF VAN NESS
  B(1)=  8.104729      B(2)=  0.005281
 B(3)=  0.003732       B(4)=  0.000107
  X           XCH2          Y                YPRED        DEVP.

 0.0100      0.9983       201.4      200.0         0.7
 0.0200      0.9966       323.2      319.1         1.3
 0.0300      0.9949       397.5      402.6        -1.3
 0.0400      0.9932       452.0      467.1        -3.3
 0.0500      0.9915       495.4      519.9        -4.9
 0.0750      0.9870       576.5      622.3        -7.9
 0.1000      0.9825       637.2      700.1        -9.9
 0.1250      0.9778       683.6      762.8       -11.6
 0.1500      0.9730       722.9      814.5       -12.7
 0.1750      0.9680       753.6      857.5       -13.8
 0.2000      0.9630       779.2      893.1       -14.6
 0.3000      0.9412       831.6      975.5       -17.3
 0.4000      0.9167       830.4      980.8       -18.1
 0.5000      0.8889       790.0      924.3       -17.0
 0.6000      0.8571       712.8      816.2       -14.5
 0.7000      0.8205       604.8      664.2        -9.8
 0.8000      0.7778       459.2      474.4        -3.3
 0.9000      0.7273       263.7      251.6         4.6
                                         RMS DEVIATION=        10.9
```

TABLE A72:

```
HEATS OF MIXING OF SYSTEM ETHANOL + HEPTANE AT 45 DEG. C
X=MOL.FRACT. OF ALCOHOL, DATA OF VAN NESS
    B(1)=  8.104729      B(2)=   0.005281
   B(3)=  0.003752       B(4)=   0.000107
    X           XCH2         Y          YPRED       DEVP

   0.0093      0.9987      194.0      196.5       -1.3
   0.0150      0.9978      284.0      279.1        1.7
   0.0199      0.9971      345.0      336.7        2.4
   0.0268      0.9961      407.0      403.7        0.8
   0.0384      0.9944      483.0      492.1       -1.9
   0.0533      0.9921      550.0      578.9       -5.3
   0.0729      0.9891      619.0      667.0       -7.8
   0.0946      0.9857      678.0      744.2       -9.8
   0.1207      0.9815      733.0      819.0      -11.7
   0.1793      0.9715      819.0      942.0      -15.0
   0.2463      0.9591      877.0     1030.6      -17.5
   0.3569      0.9360      909.0     1088.1      -19.7
   0.4695      0.9083      881.0     1054.9      -19.7
   0.5755      0.8775      810.0      952.3      -17.6
   0.6673      0.8459      716.0      814.5      -13.8
   0.7079      0.8302      663.0      740.3      -11.7
   0.7785      0.7997      557.0      593.3       -6.5
   0.8632      0.7567      396.0      388.9        1.8
   0.9444      0.7069      185.0      166.3       10.1
                                   RMS DEVIATION=          11.3
```

TABLE A73:

```
HEATS OF MIXING AT 45 DEG. C FOR SYSTEM ETHANOL + NONANE
X=MOL.FRACT. OF ALCOHOL, DATA OF VAN NESS
    B(1)=  8.104729      B(2)=   0.005281
   B(3)=  0.003732       B(4)=   0.000107
    X           XCH2        Y            YPRED       DEVP

   0.0100     0.9989      208.1        219.4         -5.4
   0.0200     0.9977      355.5        367.4         -3.3
   0.0300     0.9966      450.8        476.8         -5.8
   0.0400     0.9954      519.2        562.8         -8.4
   0.0500     0.9943      573.8        633.5        -10.4
   0.7500     0.8333     1822.5        809.3         55.6
   0.1000     0.9881      745.2        870.6        -16.8
   0.1250     0.9848      800.6        951.3        -18.8
   0.1500     0.9815      846.6       1017.9        -20.2
   0.1750     0.9780      882.1       1073.8        -21.7
   0.2000     0.9744      912.0       1121.0        -22.9
   0.3000     0.9583      980.7       1241.0        -26.5
   0.4000     0.9394      991.2       1272.0        -28.3
   0.5000     0.9167      955.0       1226.0        -28.4
   0.6000     0.8889      880.8       1109.2        -25.9
   0.7000     0.8542      766.5        925.4        -20.7
   0.8000     0.8095      601.6        677.6        -12.6
   0.9000     0.7500      368.1        368.4         -0.1
                                    RMS DEVIATION=         22.3
```

TABLE A74:

```
HEATS OF MIXING OF THE SYSTEM PROPANOL + HEPTANE AT 45 DEG. C
X=MOL.FRACT. OF ALCOHOL, DATA OF VAN NESS
     B(1)=   8.104729      B(2)=    0.005281
    B(3)=  0.003732       B(4)=    0.000107
     X          XCH2          Y           YPRED      DEVP

    0.0100     0.9986      205.5       203.8        0.8
    0.0200     0.9971      347.3       330.0        5.0
    0.0300     0.9957      438.5       419.2        4.4
    0.0400     0.9942      506.1       487.7        3.6
    0.0500     0.9927      553.4       543.2        1.8
    0.0750     0.9889      646.6       648.7       -0.3
    0.1000     0.9851      720.0       726.6       -0.9
    0.1250     0.9811      777.7       788.0       -1.3
    0.1500     0.9771      823.6       837.8       -1.7
    0.1750     0.9730      859.0       878.6       -2.3
    0.2000     0.9688      889.6       912.0       -2.5
    0.3000     0.9508      957.6       986.6       -3.0
    0.4000     0.9310      957.6       986.8       -3.1
    0.5000     0.9091      900.0       927.6       -3.1
    0.6000     0.8846      796.8       818.3       -2.7
    0.7000     0.8571      657.3       665.8       -1.3
    0.8000     0.8261      476.8       475.7        0.2
    0.9000     0.7907      258.3       252.5        2.2
                                         RMS DEVIATION=         2.6
```

TABLE A75:

```
HEATS OF MIXING AT 45 DEG. C FOR THE SYSTEM BUTANOL+HEPTANE
X=MOL.FRACT. OF ALCOHOL, DATA OF VAN NESS
    B(1)=   8.104729      B(2)=   0.005281
   B(3)=   0.003732       B(4)=   0.000107
    X            XCH2          Y            YPRED       DEVP

  0.0100       0.9986       203.1        200.3          1.4
  0.0200       0.9971       340.6        323.2          5.1
  0.0300       0.9957       430.4        409.3          4.9
  0.0400       0.9942       497.7        474.8          4.6
  0.0500       0.9928       547.2        527.5          3.6
  0.0750       0.9891       645.2        626.1          3.0
  0.1000       0.9853       701.1        697.5          0.5
  0.1250       0.9815       747.0        752.7         -0.8
  0.1500       0.9776       787.9        796.6         -1.1
  0.1750       0.9737       822.9        831.8         -1.1
  0.2000       0.9697       854.4        859.9         -0.6
  0.3000       0.9531       921.9        917.2          0.5
  0.4000       0.9355       921.6        906.6          1.6
  0.5000       0.9167       865.0        843.6          2.5
  0.6000       0.8966       760.8        737.5          3.1
  0.7000       0.8750       611.1        595.3          2.6
  0.8000       0.8519       430.4        422.3          1.9
  0.9000       0.8269       225.0        222.7          1.0
                                      RMS DEVIATION=          2.7
```

TABLE A76:

```
HEATS OF MIXING OF SYSTEM OCTANOL + HEPTANE AT 45 DEG. C
X=MOL.FRACT. OF ALCOHOL, DATA OF VAN NESS
    B(1)=  8.104729     B(2)=  0.005281
    B(3)=  0.003732     B(4)=  0.000107
     X          XCH2          Y           YPRED       DEVP

   0.0100     0.9986      195.9       189.8        3.1
   0.0200     0.9972      322.4       302.9        6.1
   0.0300     0.9958      399.8       380.0        5.0
   0.0400     0.9944      451.6       436.9        3.2
   0.0500     0.9930      491.1       481.4        2.0
   0.0750     0.9895      562.6       560.9        0.3
   0.1000     0.9861      610.2       614.4       -0.7
   0.1250     0.9828      643.1       652.8       -1.5
   0.1500     0.9795      666.8       681.0       -2.1
   0.1750     0.9762      685.8       701.7       -2.3
   0.2000     0.9730      699.2       716.3       -2.4
   0.3000     0.9605      718.2       731.2       -1.8
   0.4000     0.9487      698.4       697.0        0.2
   0.5000     0.9375      642.5       628.9        2.1
   0.6000     0.9268      554.4       535.5        3.4
   0.7000     0.9167      443.1       422.4        4.7
   0.8000     0.9070      307.2       293.6        4.4
   0.9000     0.8977      156.6       152.0        2.9
                                  RMS DEVIATION=         3.1
```

TABLE A77:

```
HEATS OF MIXING OF SYSTEM OCTANOL+NONANE AT 45 DEG. C
X=MOL.FRACT. OF ALCOHCL, DATA OF VAN NESS
    B(1)=  0.104729     B(2)=  0.005281
   B(3)=  0.003732      B(4)=  0.000107
    X          XCH2        Y            YPRED       DEVP

   0.0100     0.9989      200.1        201.2        -0.6
   0.0200     0.9978      346.3        331.9         4.2
   0.0300     0.9967      439.7        425.0         3.3
   0.0400     0.9956      500.4        495.5         1.0
   0.0500     0.9944      543.9        551.2        -1.4
   0.0750     0.9917      628.5        651.5        -3.6
   0.1000     0.9889      687.6        719.2        -4.6
   0.1250     0.9861      729.5        767.9        -5.3
   0.1500     0.9833      759.9        804.1        -5.8
   0.1750     0.9806      784.0        831.0        -6.0
   0.2000     0.9778      801.6        850.7        -6.1
   0.3000     0.9667      831.6        877.5        -5.5
   0.4000     0.9556      816.0        845.6        -3.6
   0.5000     0.9444      762.5        771.3        -1.2
   0.6000     0.9333      676.8        663.7         1.9
   0.7000     0.9222      552.3        528.8         4.3
   0.8000     0.9111      392.0        371.0         5.3
   0.9000     0.9000      205.2        193.9         5.5
                                        RMS DEVIATION=        4.3
```

TABLE A78:

HEATS OF MIXING OF SYSTEM N-PENTANOL - N-HEXANE

LAMDA CH2/OH= 0.800720 01   LAMDA PRIME CH2/OH= 0.454180-02
LAMDA OH/CH2= 0.203032-02   LAMDA PRIME OH/CH2= 0.684190-04

X ALC	X CH2	DEL H EXP	DEL H PRED	DEVIATION
0.0205	0.9966	229.8	219.9	4.310
0.0459	0.9924	311.3	306.1	1.673
0.0880	0.9853	385.4	384.4	0.262
0.1277	0.9787	431.8	432.9	-0.263
0.1637	0.9727	462.5	464.9	-0.515
0.1962	0.9673	484.8	486.2	-0.295
0.2269	0.9622	501.8	500.9	0.179
0.2551	0.9575	512.8	510.2	0.499
0.2815	0.9531	521.4	515.7	1.085
0.3058	0.9490	525.9	518.3	1.449
0.3291	0.9452	529.0	518.6	1.968
0.3506	0.9416	529.1	517.2	2.257
0.3707	0.9382	527.5	514.4	2.480
0.3896	0.9351	524.5	510.7	2.637
0.4072	0.9321	519.7	506.2	2.596
0.4243	0.9293	515.4	501.0	2.790
0.4404	0.9266	509.5	495.4	2.769
0.4554	0.9241	503.2	489.5	2.717
0.4700	0.9217	496.5	483.3	2.666
0.4835	0.9194	489.4	477.0	2.533
0.4962	0.9173	482.1	470.7	2.361
0.5107	0.9149	473.5	463.1	2.201
0.5224	0.9129	465.6	456.6	1.940
0.5318	0.9114	458.8	451.1	1.674
0.5325	0.9112	458.3	450.7	1.657
0.5410	0.9098	452.2	445.6	1.459
0.5423	0.9096	451.6	444.8	1.503
0.5504	0.9083	445.7	439.8	1.327
0.5527	0.9079	443.3	438.3	1.120
0.5595	0.9068	439.0	434.0	1.144
0.5632	0.9061	435.6	431.6	0.926
0.5746	0.9042	426.3	424.0	0.546
0.5858	0.9024	417.0	416.3	0.176
0.5980	0.9003	406.7	407.6	-0.220
0.6109	0.8982	396.1	398.2	-0.531
0.6238	0.8960	384.1	388.4	-1.108
0.6371	0.8938	372.0	378.0	-1.607
0.6509	0.8915	359.1	366.9	-2.169
0.6652	0.8891	345.8	355.1	-2.678
0.6805	0.8866	331.0	342.0	-3.335
0.6964	0.8839	315.2	328.1	-4.098
0.7131	0.8812	298.7	313.1	-4.814
0.7308	0.8782	280.7	296.7	-5.699
0.7493	0.8751	262.0	279.1	-6.524
0.7688	0.8719	241.8	260.0	-7.532
0.7897	0.8684	219.7	239.0	-8.802
0.8107	0.8649	198.3	217.4	-9.624
0.8335	0.8611	173.5	193.3	-11.391
0.8576	0.8571	148.6	167.1	-12.451
0.8825	0.8529	122.5	139.4	-13.782
0.9104	0.8483	93.0	107.5	-15.625
0.9375	0.8438	65.4	75.8	-15.940
0.9688	0.8385	32.4	38.3	-18.232

RMS DEVIATION = 5.8191

TABLE A79:

HEATS OF MIXING OF SYSTEM N-PENTANOL - 2,2-DIMETHYLBUTANE

LAMDA CH2/OH= 0.80072D 01   LAMDA PRIME CH2/OH= 0.45418D-02
LAMDA OH/CH2= 0.20303D-02   LAMDA PRIME OH/CH2= 0.66419D-04

X ALC	X CH2	DEL H EXP	DEL H PRED	DEVIATION
0.0196	0.9967	221.4	215.3	2.740
0.0458	0.9924	304.9	305.8	-0.310
0.0887	0.9952	376.5	385.4	-2.364
0.1280	0.9787	418.8	433.2	-3.449
0.1644	0.9726	448.0	465.4	-3.887
0.1975	0.9671	469.2	487.0	-3.783
0.2277	0.9621	483.9	501.2	-3.579
0.2559	0.9574	494.4	510.5	-3.246
0.2820	0.9530	501.3	515.8	-2.897
0.3065	0.9489	505.5	518.3	-2.535
0.3298	0.9450	507.5	518.6	-2.181
0.3516	0.9414	507.0	517.1	-1.983
0.3726	0.9379	504.9	514.1	-1.821
0.3919	0.9347	501.0	510.1	-1.824
0.4110	0.9315	495.8	505.1	-1.881
0.4281	0.9287	490.3	499.8	-1.928
0.4442	0.9260	483.4	494.0	-2.184
0.4597	0.9234	476.8	487.7	-2.294
0.4738	0.9210	469.3	481.5	-2.610
0.4876	0.9187	462.3	475.0	-2.751
0.5000	0.9167	454.3	468.8	-3.183
0.5123	0.9146	447.1	462.2	-3.378
0.5233	0.9128	439.1	456.1	-3.861
0.5318	0.9114	436.8	451.1	-3.278
0.5367	0.9105	430.7	448.2	-4.064
0.5472	0.9088	423.0	441.8	-4.441
0.5418	0.9097	429.7	445.1	-3.588
0.5518	0.9080	422.5	438.9	-3.882
0.5574	0.9071	415.6	435.3	-4.748
0.5622	0.9063	413.9	432.2	-4.427
0.5732	0.9045	405.6	424.9	-4.763
0.5844	0.9026	397.0	417.2	-5.099
0.5961	0.9007	387.1	409.0	-5.648
0.6085	0.8986	376.3	399.9	-6.275
0.6217	0.8964	365.0	390.0	-6.840
0.6353	0.8941	352.6	379.4	-7.601
0.6491	0.8918	340.4	368.4	-8.212
0.6637	0.8894	326.8	356.3	-9.032
0.6794	0.8868	311.8	343.0	-10.002
0.6954	0.8841	296.9	329.0	-10.813
0.7119	0.8814	281.0	314.2	-11.806
0.7294	0.8784	264.3	298.0	-12.754
0.7477	0.8754	246.2	280.6	-13.986
0.7672	0.8721	227.0	261.6	-15.249
0.7878	0.8687	207.0	241.0	-16.411
0.8092	0.8651	186.3	218.9	-17.525
0.8320	0.8613	163.9	194.9	-18.896
0.8558	0.8574	140.2	169.1	-20.598
0.8814	0.8531	114.6	140.6	-22.707
0.9081	0.8487	88.8	110.2	-24.085
0.9365	0.8439	60.9	77.0	-26.449
0.9672	0.8388	31.4	40.2	-28.177

RMS DEVIATION = 10.3412

TABLE A80:

HEATS OF MIXING OF SYSTEM N-PENTANOL - 2,3-DIMETHYLBUTANE

LAMDA CH2/OH= 0.80072D 01 LAMDA PRIME CH2/OH= 0.45418D-02
LAMDA OH/CH2= 0.20303D-02 LAMDA PRIME OH/CH2= 0.66419D-04

X ALC	X CH2	DEL H EXP	DEL H PRED	DEVIATION
0.0217	0.9964	233.6	225.7	3.376
0.0452	0.9925	305.5	304.4	0.374
0.0877	0.9854	377.5	384.0	-1.709
0.1270	0.9788	420.4	432.2	-2.810
0.1627	0.9729	449.9	464.1	-3.161
0.1959	0.9674	471.5	486.1	-3.089
0.2268	0.9622	486.4	500.9	-2.973
0.2553	0.9575	497.6	510.3	-2.551
0.2818	0.9530	505.0	515.8	-2.137
0.3070	0.9488	509.0	518.3	-1.836
0.3341	0.9443	508.8	518.4	-1.887
0.3551	0.9408	509.3	516.7	-1.445
0.3757	0.9374	506.7	513.5	-1.349
0.3942	0.9343	502.5	509.6	-1.412
0.4114	0.9314	497.9	505.0	-1.428
0.4279	0.9287	492.4	499.8	-1.507
0.4435	0.9261	486.1	494.2	-1.672
0.4581	0.9237	479.8	488.4	-1.794
0.4723	0.9213	472.2	482.2	-2.124
0.4855	0.9191	465.2	476.0	-2.330
0.4984	0.9169	457.7	469.6	-2.597
0.5110	0.9148	449.9	462.9	-2.893
0.5231	0.9128	441.9	456.2	-3.229
0.5327	0.9112	434.8	450.6	-3.631
0.5342	0.9110	432.7	449.7	-3.928
0.5423	0.9096	428.0	444.8	-3.928
0.5439	0.9094	425.7	443.8	-4.259
0.5515	0.9081	421.4	439.1	-4.198
0.5540	0.9077	417.9	437.5	-4.692
0.5647	0.9059	409.7	430.6	-5.097
0.5759	0.9040	400.8	423.1	-5.562
0.5870	0.9022	391.6	415.4	-6.084
0.5988	0.9002	381.5	407.0	-6.689
0.6108	0.8982	371.3	398.2	-7.245
0.6238	0.8960	359.9	388.4	-7.907
0.6371	0.8938	348.0	378.0	-8.614
0.6511	0.8915	335.7	366.7	-9.242
0.6656	0.8891	321.9	354.7	-10.197
0.6807	0.8866	307.3	341.9	-11.248
0.6958	0.8840	293.4	328.6	-12.014
0.7122	0.8813	277.6	313.9	-13.077
0.7296	0.8784	260.8	297.8	-14.195
0.7478	0.8754	243.2	280.5	-15.353
0.7681	0.8720	222.7	260.7	-17.074
0.7880	0.8687	203.1	240.8	-18.546
0.8089	0.8652	183.0	219.3	-19.816
0.8313	0.8615	160.7	195.6	-21.729
0.8552	0.8575	137.4	169.7	-23.535
0.8807	0.8532	112.6	141.4	-25.586
0.9077	0.8487	86.6	110.6	-27.771
0.9373	0.8438	58.5	76.1	-30.019
0.9669	0.8389	30.1	40.6	-34.921

RMS DEVIATION = 11.7827

TABLE A81:

HEATS OF MIXING OF SYSTEM N-PENTANOL - 2-METHYLPENTANE

LAMDA CH2/OH= 0.80072D 01 LAMDA PRIME CH2/OH= 0.45419D-02
LAMDA OH/CH2= 0.20303D-02 LAMDA PRIME OH/CH2= 0.66419D-04

X ALC	X CH2	DEL H EXP	DEL H PRED	DEVIATION
0.0194	0.9968	213.6	214.3	-0.325
0.0446	0.9926	295.2	302.9	-2.592
0.0862	0.9856	368.1	381.8	-3.709
0.1249	0.9792	413.3	429.9	-4.021
0.1612	0.9731	444.0	463.0	-4.272
0.1941	0.9677	466.5	495.0	-3.974
0.2247	0.9626	483.1	500.0	-3.500
0.2532	0.9578	494.9	509.7	-3.017
0.2795	0.9534	502.4	515.4	-2.594
0.3040	0.9493	508.0	518.2	-2.002
0.3273	0.9455	510.4	519.6	-1.614
0.3487	0.9419	510.6	517.3	-1.322
0.3684	0.9386	509.3	514.8	-1.080
0.3878	0.9354	506.7	511.1	-0.864
0.4063	0.9323	502.3	506.5	-0.828
0.4237	0.9294	497.4	501.2	-0.767
0.4397	0.9267	491.8	495.6	-0.783
0.4557	0.9241	485.7	489.6	-0.805
0.4701	0.9216	479.6	483.2	-0.965
0.4841	0.9193	471.3	476.7	-1.149
0.4975	0.9171	463.5	470.1	-1.413
0.5096	0.9151	456.3	463.7	-1.616
0.5207	0.9132	449.3	457.5	-1.832
0.5314	0.9114	442.2	451.4	-2.071
0.5324	0.9113	447.4	450.8	-0.752
0.5421	0.9097	435.0	444.9	-2.283
0.5472	0.9096	440.6	444.9	-0.970
0.5516	0.9081	428.0	439.0	-2.577
0.5524	0.9079	433.0	438.5	-1.276
0.5630	0.9062	424.7	431.7	-1.648
0.5739	0.9044	416.0	424.4	-2.031
0.5855	0.9024	406.6	416.5	-2.429
0.5974	0.9004	396.2	408.0	-2.985
0.6098	0.8984	386.3	399.9	-3.274
0.6230	0.8962	374.6	389.0	-3.837
0.6363	0.8940	362.2	379.6	-4.531
0.6504	0.8916	349.5	367.3	-5.092
0.6650	0.8892	335.9	355.2	-5.754
0.6803	0.8866	321.2	342.2	-6.542
0.6961	0.8840	306.0	328.4	-7.315
0.7129	0.8812	289.4	313.3	-8.245
0.7301	0.8783	272.3	297.4	-9.200
0.7486	0.8752	253.6	277.8	-10.319
0.7675	0.8721	234.7	261.3	-11.341
0.7873	0.8688	214.7	241.5	-12.472
0.8087	0.8652	193.4	219.5	-13.480
0.8315	0.8614	169.6	195.4	-15.215
0.8563	0.8573	145.6	168.5	-15.743
0.8815	0.8531	119.5	140.5	-17.581
0.9078	0.8487	92.8	110.5	-19.110
0.9366	0.8439	6[illegible].3	76.9	-1[illegible]79
0.9668	0.8389	33.4	40.7	-21.953

RMS DEVIATION = 7.7313

TABLE A82:

HEATS OF MIXING OF SYSTEM N-PENTANOL - 3-METHYLPENTANE

LAMDA CH2/OH= 0.80072D 01 LAMDA PRIME CH2/OH= 0.4[illegible]4190-02
LAMDA OH/CH2= 0.20303D-02 LAMDA PRIME OH/CH2= 0.66419D-04

X ALC	X CH2	DEL H EXP	DEL H PRED	DEVIATION
0.0206	0.9966	226.6	220.4	2.739
0.0446	0.9926	303.7	302.9	0.279
0.0860	0.9857	375.9	381.5	-1.478
0.1257	0.9791	421.2	430.9	-2.294
0.1618	0.9730	452.1	463.4	-2.506
0.1944	0.9676	474.3	485.2	-2.300
0.2251	0.9625	489.9	500.2	-2.097
0.2539	0.9577	501.3	509.9	-1.714
0.2808	0.9532	509.9	515.6	-1.125
0.3061	0.9490	514.1	518.3	-0.816
0.3293	0.9451	516.6	518.6	-0.384
0.3513	0.9415	515.9	517.1	-0.230
0.3709	0.9382	514.5	514.4	0.022
0.3934	0.9344	509.4	509.8	-0.076
0.4105	0.9316	505.8	505.3	0.104
0.4274	0.9288	500.5	500.0	0.102
0.4431	0.9262	494.3	494.4	-0.016
0.4576	0.9237	487.9	488.6	-0.147
0.4711	0.9215	480.9	482.8	-0.410
0.4842	0.9193	473.8	476.7	-0.605
0.4965	0.9173	466.7	470.6	-0.828
0.5090	0.9152	459.3	464.0	-1.023
0.5160	0.9140	457.9	460.2	-0.495
0.5204	0.9133	451.6	457.7	-1.351
0.5259	0.9123	451.2	454.6	-0.745
0.5315	0.9114	444.4	451.3	-1.552
0.5361	0.9107	443.7	448.6	-1.096
0.5422	0.9096	436.6	444.9	-1.895
0.5468	0.9089	434.8	442.0	-1.664
0.5515	0.9081	429.5	439.1	-2.233
0.5576	0.9071	426.1	435.2	-2.137
0.5689	0.9052	417.6	427.9	-2.459
0.5808	0.9032	407.2	419.7	-3.079
0.5933	0.9011	396.4	411.0	-3.675
0.6064	0.8989	384.9	401.5	-4.304
0.6198	0.8967	372.5	391.4	-5.079
0.6340	0.8943	359.9	380.4	-5.703
0.6490	0.8918	345.1	368.4	-6.761
0.6646	0.8892	331.0	355.6	-7.421
0.6812	0.8865	315.2	341.4	-8.323
0.6982	0.8836	299.0	326.5	-9.203
0.7163	0.8806	281.1	310.2	-10.335
0.7353	0.8775	262.5	292.5	-11.413
0.7549	0.8742	242.4	273.7	-12.901
0.7760	0.8707	221.3	252.9	-14.262
0.7984	0.8669	199.1	230.1	-15.588
0.8222	0.8630	175.1	205.3	-17.245
0.8467	0.8589	150.4	179.0	-19.028
0.8728	0.8545	124.4	150.3	-20.790
0.9027	0.8496	95.3	117.0	-22.747
0.9333	0.8444	64.7	80.8	-24.863
0.9651	0.8392	32.9	42.9	-30.063

RMS DEVIATION = 9.2002

```
HEATS OF MIXING OF SYSTEM ISOPENTANOL - N-HEXANE

LAMDA CH2/OH= 0.80072D 01      LAMDA PRIME CH2/OH= 0.45418D-02
LAMDA OH/CH2= 0.20303D-02      LAMDA PRIME OH/CH2= 0.66419D-04

  X ALC       X CH2   DEL H EXP DEL H PRED  DEVIATION
0.0212      0.9965     238.7      223.3      6.441
0.0449      0.9925     316.9      303.6      4.195
0.0869      0.9855     395.3      382.8      3.166
0.1257      0.9791     445.3      430.9      3.242
0.1617      0.9731     481.0      463.4      3.669
0.1943      0.9676     506.6      485.2      4.234
0.2243      0.9626     526.6      499.8      5.080
0.2529      0.9579     542.3      509.6      6.022
0.2793      0.9535     553.7      515.4      6.917
0.3040      0.9493     561.5      518.2      7.717
0.3269      0.9455     566.9      518.6      8.512
0.3484      0.9419     569.4      517.4      9.136
0.3687      0.9386     570.3      514.8      9.740
0.3878      0.9354     569.7      511.1     10.290
0.4057      0.9324     567.4      506.6     10.711
0.4225      0.9296     563.8      501.6     11.032
0.4384      0.9269     559.8      496.1     11.374
0.4536      0.9244     554.9      490.3     11.649
0.4685      0.9219     548.4      483.9     11.756
0.4819      0.9197     542.8      477.8     11.981
0.4948      0.9175     536.3      471.4     12.096
0.5068      0.9155     529.2      465.2     12.098
0.5183      0.9136     522.6      458.9     12.192
0.5291      0.9118     515.4      452.7     12.164
0.5360      0.9107     506.8      448.6     11.479
0.5396      0.9101     508.8      446.5     12.253
0.5456      0.9091     500.0      442.9     11.444
0.5499      0.9083     501.3      440.1     12.208
0.5556      0.9074     492.8      436.5     11.427
0.5661      0.9057     484.6      429.7     11.337
0.5771      0.9038     475.7      422.3     11.231
0.5887      0.9019     466.0      414.2     11.109
0.6007      0.8999     455.4      405.6     10.927
0.6130      0.8978     444.5      396.6     10.785
0.6258      0.8957     432.7      386.8     10.604
0.6390      0.8935     419.6      376.5     10.279
0.6529      0.8912     406.1      365.3     10.058
0.6677      0.8887     391.0      353.0      9.729
0.6831      0.8862     375.4      339.8      9.486
0.6993      0.8835     358.3      325.5      9.144
0.7157      0.8807     340.2      310.7      8.671
0.7330      0.8778     320.9      294.6      8.187
0.7512      0.8748     299.7      277.3      7.489
0.7702      0.8716     278.4      258.6      7.097
0.7903      0.8683     254.9      238.4      6.462
0.8114      0.8648     221.4      216.1      5.556
0.8341      0.8610     202.6      192.6      4.926
0.8583      0.8569     173.2      166.3      3.965
0.8829      0.8529     143.8      138.9      3.385
0.9107      0.8482     109.6      107.2      2.204
0.9384      0.8436      75.3       74.8      0.719
0.9684      0.8386      39.4       39.8     -1.022

RMS DEVIATION =     9.0752
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TABLE A84:

HEATS OF MIXING OF SYSTEM ISOPENTANOL - 2,2-DIMETHYLBUTANE

LAMDA CH2/OH= 0.80072D 01 LAMDA PRIME CH2/OH= 0.45418D-02
LAMDA OH/CH2= 0.20303D-02 LAMDA PRIME OH/CH2= 0.66419D-04

X ALC	X CH2	DEL H EXP	DEL H PRED	DEVIATION
0.0216	0.9964	232.3	225.2	3.039
0.0462	0.9923	309.8	306.8	0.959
0.0887	0.9852	383.3	385.4	-0.548
0.1291	0.9785	428.6	434.4	-1.346
0.1658	0.9724	460.0	466.5	-1.404
0.1991	0.9668	482.8	487.8	-1.042
0.2298	0.9617	500.2	502.0	-0.367
0.2590	0.9568	511.8	511.2	0.109
0.2862	0.9523	520.6	516.4	0.803
0.3105	0.9483	526.2	518.5	1.463
0.3333	0.9445	529.8	518.4	2.145
0.3541	0.9410	530.9	516.8	2.660
0.3739	0.9377	530.4	513.9	3.118
0.3925	0.9346	527.8	510.0	3.373
0.4099	0.9317	524.8	505.4	3.688
0.4264	0.9289	520.8	500.3	3.932
0.4424	0.9263	515.8	494.6	4.102
0.4576	0.9237	509.8	488.6	4.155
0.4713	0.9215	504.1	482.7	4.249
0.4844	0.9193	497.8	476.6	4.265
0.4971	0.9172	491.1	470.3	4.244
0.5094	0.9151	484.0	463.8	4.177
0.5213	0.9131	477.2	457.2	4.193
0.5321	0.9113	469.6	450.9	3.973
0.5441	0.9093	457.0	443.7	2.909
0.5448	0.9092	461.0	443.3	3.845
0.5540	0.9077	449.3	437.5	2.625
0.5552	0.9075	453.7	436.7	3.737
0.5643	0.9060	441.1	430.8	2.324
0.5750	0.9042	433.8	423.7	2.328
0.5866	0.9022	423.7	415.7	1.887
0.5981	0.9003	414.3	407.5	1.636
0.6103	0.8983	403.3	398.6	1.172
0.6234	0.8961	391.6	388.7	0.750
0.6363	0.8940	377.2	378.6	-0.374
0.6529	0.8912	364.3	365.3	-0.262
0.6677	0.8887	350.7	353.0	-0.644
0.6823	0.8863	335.5	340.5	-1.485
0.6986	0.8836	318.8	326.2	-2.309
0.7149	0.8809	302.3	311.4	-3.022
0.7328	0.8779	283.4	294.8	-4.028
0.7509	0.8749	263.9	277.5	-5.172
0.7699	0.8717	244.0	258.9	-6.123
0.7909	0.8682	222.6	237.8	-6.836
0.8123	0.8646	198.5	215.7	-8.671
0.8341	0.8610	175.4	192.6	-9.818
0.8577	0.8571	149.8	167.0	-11.477
0.8835	0.8528	122.5	138.3	-12.862
0.9096	0.8484	94.9	108.6	-14.284
0.9385	0.8436	63.9	74.6	-16.808
0.9690	0.8385	31.6	38.1	-20.457

RMS DEVIATION = 5.9419

```
HEATS OF MIXING OF SYSTEM ISOPENTANOL - 2,3-DIMETHYLBUTANE

LAMDA CH2/OH= 0.80072D 01      LAMDA PRIME CH2/OH= 0.45418D-02
LAMDA OH/CH2= 0.20303D-02      LAMDA PRIME OH/CH2= 0.66419D-04

  X ALC      X CH2   DEL H EXP DEL H PRED  DEVIATION
 0.0200     0.9967     217.3     217.4      -0.039
 0.0449     0.9925     297.5     303.6      -2.082
 0.0860     0.9857     371.5     381.5      -2.680
 0.1262     0.9790     419.7     431.4      -2.784
 0.1614     0.9731     451.8     463.1      -2.506
 0.1947     0.9676     475.5     485.4      -2.078
 0.2251     0.9625     494.3     500.2      -1.188
 0.2531     0.9578     507.7     509.7      -0.394
 0.2786     0.9536     517.1     515.3       0.351
 0.3032     0.9495     524.5     518.1       1.217
 0.3264     0.9456     529.0     518.7       1.956
 0.3476     0.9421     530.1     517.5       2.386
 0.3675     0.9388     531.1     514.9       3.042
 0.3867     0.9356     529.7     511.3       3.470
 0.4048     0.9325     527.3     506.9       3.874
 0.4248     0.9292     521.6     500.9       3.977
 0.4410     0.9265     517.7     495.2       4.353
 0.4546     0.9242     512.1     489.9       4.344
 0.4687     0.9219     506.7     483.8       4.511
 0.4818     0.9197     500.3     477.8       4.494
 0.4950     0.9175     493.6     471.3       4.513
 0.5065     0.9156     487.1     465.3       4.467
 0.5177     0.9137     480.4     459.2       4.409
 0.5286     0.9119     473.5     453.0       4.330
 0.5317     0.9114     472.7     451.2       4.553
 0.5386     0.9102     466.4     447.1       4.147
 0.5415     0.9098     465.8     445.3       4.401
 0.5482     0.9086     459.8     441.2       4.053
 0.5519     0.9080     458.2     438.8       4.225
 0.5628     0.9062     450.0     431.8       4.038
 0.5736     0.9044     441.6     424.7       3.838
 0.5850     0.9025     431.9     416.8       3.491
 0.5968     0.9005     421.9     408.5       3.186
 0.6092     0.8985     410.8     399.4       2.777
 0.6222     0.8963     399.0     389.6       2.360
 0.6357     0.8941     386.1     379.1       1.817
 0.6500     0.8917     372.3     367.6       1.257
 0.6648     0.8892     358.2     355.4       0.783
 0.6793     0.8868     343.6     343.1       0.153
 0.6957     0.8841     326.8     328.7      -0.593
 0.7124     0.8813     309.8     313.7      -1.265
 0.7302     0.8783     290.8     297.3      -2.221
 0.7486     0.8752     271.5     279.8      -3.045
 0.7680     0.8720     250.2     260.9      -4.245
 0.7887     0.8686     227.3     240.1      -5.612
 0.8108     0.8649     203.7     217.3      -6.667
 0.8332     0.8611     179.3     193.6      -7.967
 0.8575     0.8571     152.5     167.2      -9.647
 0.8830     0.8528     124.7     138.8     -11.323
 0.9097     0.8484      95.3     108.3     -13.683
 0.9377     0.8437      65.5      75.6     -15.401
 0.9678     0.8387      32.4      39.5     -21.976

RMS DEVIATION =     5.7469
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TABLE A86:

HEATS OF MIXING OF SYSTEM ISOPENTANOL - 2-METHYLPENTANE

LAMDA CH2/OH= 0.800720 01   LAMDA PRIME CH2/OH= 0.45418D-02
LAMDA OH/CH2= 0.20303D-02   LAMDA PRIME OH/CH2= 0.66419D-04

X ALC	X CH2	DEL H EXP	DEL H PRED	DEVIATION
0.0217	0.9964	241.9	225.7	6.691
0.0462	0.9923	319.4	306.8	3.936
0.0886	0.9852	395.7	385.3	2.639
0.1281	0.9787	442.2	433.3	2.002
0.1649	0.9725	475.4	465.8	2.022
0.1984	0.9669	498.7	487.4	2.256
0.2291	0.9618	517.1	501.8	2.966
0.2578	0.9570	531.1	510.9	3.796
0.2839	0.9527	540.2	516.1	4.461
0.3091	0.9485	547.0	518.4	5.220
0.3317	0.9447	550.0	518.5	5.727
0.3533	0.9411	551.6	516.9	6.296
0.3730	0.9378	551.8	514.0	6.846
0.3918	0.9347	549.8	510.2	7.209
0.4098	0.9317	547.1	505.5	7.609
0.4265	0.9289	543.1	500.3	7.882
0.4423	0.9263	538.0	494.7	8.052
0.4576	0.9237	532.7	488.6	8.275
0.4718	0.9214	526.0	482.5	8.279
0.4847	0.9192	519.6	476.4	8.309
0.4977	0.9171	513.1	469.9	8.410
0.5102	0.9150	506.1	463.3	8.447
0.5220	0.9130	498.5	456.8	8.366
0.5331	0.9112	491.1	450.4	8.297
0.5361	0.9107	486.9	448.6	7.873
0.5439	0.9094	484.0	443.8	8.300
0.5459	0.9090	479.8	442.6	7.754
0.5543	0.9076	[illegible]6.4	437.3	8.204
0.5560	0.9073	471.9	436.2	7.558
0.5666	0.9056	463.5	429.3	7.372
0.5779	0.9037	454.8	421.7	7.272
0.5894	0.9018	444.4	413.7	6.900
0.6012	0.8998	435.1	405.3	6.855
0.6136	0.8977	424.3	396.1	6.645
0.6267	0.8956	412.3	386.1	6.350
0.6401	0.8933	399.1	375.6	5.890
0.6540	0.8910	385.3	364.4	5.437
0.6688	0.8885	370.9	352.0	5.088
0.6847	0.8859	355.3	338.4	4.757
0.7010	0.8832	338.2	324.0	4.193
0.7177	0.8804	320.3	308.9	3.570
0.7355	0.8774	301.3	292.3	2.997
0.7540	0.8743	281.1	274.5	2.332
0.7731	0.8712	259.7	255.8	1.518
0.7931	0.8678	237.2	235.6	0.687
0.8143	0.8643	213.4	213.6	-0.102
0.8366	0.8606	187.7	189.9	-1.191
0.8608	0.8565	159.5	163.6	-2.557
0.8855	0.8524	131.5	136.0	-3.421
0.9109	0.8482	101.7	107.0	-5.165
0.9390	0.8435	69.6	74.0	-6.391
0.9688	0.8385	36.0	38.3	-6.409

RMS DEVIATION = 6.0195

TABLE A87:

HEATS OF MIXING OF SYSTEM ISOPENTANOL - 3-METHYLPENTANE

LAMDA CH2/OH= 0.80072D 01   LAMDA PRIME CH2/OH= 0.45418D-02
LAMDA OH/CH2= 0.20303D-02   LAMDA PRIME OH/CH2= 0.66419D-04

X ALC	X CH2	DEL H EXP	DEL H PRED	DEVIATION
0.0206	0.9966	225.6	220.4	2.309
0.0633	0.9895	344.3	343.5	0.226
0.1036	0.9827	404.1	405.5	-0.343
0.1406	0.9766	444.3	445.5	-0.272
0.1747	0.9709	472.9	472.8	0.014
0.2060	0.9657	495.3	491.5	0.776
0.2344	0.9609	512.3	503.8	1.669
0.2615	0.9564	524.6	511.9	2.439
0.2865	0.9523	534.0	516.5	3.285
0.3102	0.9483	540.2	518.5	4.019
0.3321	0.9447	544.0	518.5	4.690
0.3569	0.9405	544.0	516.4	5.066
0.3761	0.9373	545.5	513.5	5.873
0.3942	0.9343	544.0	509.6	6.325
0.4119	0.9313	541.3	504.9	6.731
0.4279	0.9287	537.4	499.8	6.993
0.4432	0.9261	532.7	494.3	7.236
0.4578	0.9237	527.3	488.5	7.352
0.4717	0.9214	521.5	482.5	7.478
0.4850	0.9192	514.9	476.3	7.500
0.4972	0.9171	508.2	470.2	7.477
0.5089	0.9152	502.2	464.1	7.596
0.5205	0.9133	495.0	457.6	7.546
0.5268	0.9122	487.4	454.0	6.844
0.5314	0.9114	487.6	451.4	7.433
0.5369	0.9105	480.8	448.1	6.804
0.5420	0.9097	480.5	445.0	7.389
0.5472	0.9088	473.5	441.8	6.698
0.5522	0.9080	473.8	438.6	7.419
0.5576	0.9071	464.2	435.2	6.246
0.5684	0.9053	456.2	428.1	6.152
0.5797	0.9034	446.9	420.5	5.909
0.5915	0.9014	437.0	412.2	5.664
0.6039	0.8994	426.2	403.3	5.372
0.6172	0.8971	414.4	393.4	5.069
0.6306	0.8949	402.0	383.1	4.704
0.6449	0.8925	388.1	371.7	4.243
0.6600	0.8900	373.4	359.4	3.749
0.6758	0.8874	357.5	346.1	3.195
0.6922	0.8846	341.1	331.8	2.717
0.7091	0.8818	323.4	316.7	2.065
0.7268	0.8789	304.7	300.4	1.397
0.7453	0.8758	283.9	282.9	0.338
0.7652	0.8725	262.7	263.6	-0.338
0.7856	0.8691	239.8	243.2	-1.418
0.8077	0.8654	215.9	220.5	-2.136
0.8306	0.8616	190.0	196.4	-3.351
0.8547	0.8576	162.9	170.3	-4.534
0.8808	0.8532	134.1	141.3	-5.367
0.9079	0.8487	103.4	110.4	-6.788
0.9367	0.8439	70.3	76.8	-9.205
0.9677	0.8387	35.6	39.6	-11.353

RMS DEVIATION = 5.4657

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HEATS OF MIXING OF SYSTEM ISOPENTANOL -- N-HEPTANE

    LAMDA CH2/OH= 0.80072D 01       LAMDA PRIME CH2/OH= 0.45418D-02
    LAMDA OH/CH2= 0.20303D-02       LAMDA PRIME OH/CH2= 0.66419D-04

      X ALC       X CH2   DEL H EXP DEL H PRED  DEVIATION
    0.0217      0.9969      252.4      244.7      3.070
    0.0508      0.9927      353.4      348.6      1.361
    0.0973      0.9859      441.2      436.4      1.087
    0.1395      0.9797      495.4      488.2      1.459
    0.1783      0.9739      534.2      522.4      2.202
    0.2137      0.9685      563.1      545.2      3.183
    0.2463      0.9635      584.3      560.0      4.157
    0.2758      0.9590      600.3      568.9      5.225
    0.3030      0.9548      611.8      573.7      6.225
    0.3286      0.9507      619.4      575.4      7.104
    0.3516      0.9471      624.0      574.7      7.895
    0.3744      0.9435      626.1      572.1      8.617
    0.3950      0.9402      626.7      568.2      9.327
    0.4145      0.9371      624.8      563.2      9.852
    0.4329      0.9341      621.8      557.4     10.356
    0.4501      0.9313      617.8      551.0     10.812
    0.4666      0.9286      612.3      544.0     11.149
    0.4821      0.9260      606.3      536.8     11.469
    0.4966      0.9236      599.5      529.4     11.700
    0.5104      0.9214      592.1      521.8     11.877
    0.5229      0.9193      585.2      514.5     12.086
    0.5351      0.9172      577.2      507.0     12.170
    0.5469      0.9153      570.1      499.3     12.414
    0.5572      0.9135      565.3      492.4     12.898
    0.5578      0.9134      561.4      492.0     12.367
    0.5661      0.9120      558.0      486.2     12.871
    0.5682      0.9117      553.0      484.7     12.353
    0.5762      0.9103      550.1      478.9     12.942
    0.5779      0.9100      545.6      477.7     12.453
    0.5866      0.9085      541.2      471.2     12.940
    0.5970      0.9068      532.2      463.2     12.969
    0.6083      0.9048      521.9      454.2     12.968
    0.6198      0.9029      511.0      444.9     12.952
    0.6320      0.9008      499.2      434.5     12.957
    0.6447      0.8986      486.5      423.5     12.956
    0.6578      0.8963      472.4      411.7     12.846
    0.6715      0.8939      457.2      399.1     12.718
    0.6858      0.8914      442.4      385.4     12.876
    0.7006      0.8888      424.8      370.9     12.683
    0.7158      0.8861      406.3      355.6     12.482
    0.7323      0.8832      386.5      338.5     12.431
    0.7494      0.8801      364.7      320.2     12.207
    0.7673      0.8769      341.6      300.5     12.031
    0.7861      0.8735      316.5      279.2     11.770
    0.8053      0.8700      290.0      256.9     11.401
    0.8258      0.8662      261.7      232.5     11.172
    0.8471      0.8623      230.9      206.3     10.636
    0.8697      0.8581      198.3      177.9     10.298
    0.8935      0.8537      163.4      147.1      9.974
    0.9187      0.8489      124.5      113.6      8.719
    0.9442      0.8441       86.7       78.9      8.977
    0.9717      0.8388       43.0       40.5      5.785

RMS DEVIATION =     10.6768
```

```
HEATS OF MIXING OF SYSTEM ISOPENTANOL - N-OCTANE

LAMDA CH2/OH= 0.80072D 01     LAMDA PRIME CH2/OH= 0.45418D-02
LAMDA OH/CH2= 0.20303D-02     LAMDA PRIME OH/CH2= 0.66419D-04

  X ALC       X CH2   DEL H EXP DEL H PRED  DEVIATION
0.0247      0.9969      279.3      278.6       0.247
0.0548      0.9931      383.1      388.3      -1.351
0.1056      0.9864      484.1      486.0      -0.400
0.1513      0.9803      545.2      542.0       0.586
0.1924      0.9747      588.6      577.7       1.845
0.2294      0.9696      621.2      600.8       3.282
0.2647      0.9646      644.6      615.9       4.448
0.2957      0.9601      661.7      624.2       5.666
0.3248      0.9558      673.8      628.1       6.787
0.3524      0.9517      681.7      628.5       7.811
0.3776      0.9479      686.3      626.2       8.762
0.4011      0.9443      687.7      621.9       9.572
0.4228      0.9409      686.1      616.1      10.197
0.4425      0.9378      683.4      609.5      10.812
0.4613      0.9348      679.7      602.0      11.436
0.4784      0.9321      674.1      594.1      11.866
0.4947      0.9294      667.9      585.8      12.299
0.5099      0.9270      660.9      577.2      12.661
0.5269      0.9241      652.2      566.9      13.086
0.5403      0.9219      643.4      558.1      13.261
0.5528      0.9198      635.4      549.4      13.530
0.5645      0.9178      627.0      540.9      13.726
0.5756      0.9160      618.2      532.5      13.859
0.5804      0.9151      608.6      528.8      13.115
0.5866      0.9141      609.4      523.9      14.037
0.5902      0.9135      600.9      520.9      13.305
0.5968      0.9123      600.6      515.5      14.165
0.6002      0.9117      591.9      512.7      13.382
0.6084      0.9103      590.2      505.7      14.313
0.6106      0.9099      582.4      503.8      13.492
0.6214      0.9080      572.3      494.3      13.626
0.6324      0.9061      561.0      484.3      13.667
0.6439      0.9041      548.8      473.6      13.710
0.6559      0.9019      535.9      462.0      13.796
0.6682      0.8997      522.0      449.7      13.845
0.6810      0.8974      506.9      436.6      13.867
0.6944      0.8950      490.9      422.5      13.943
0.7083      0.8924      473.6      407.3      13.992
0.7227      0.8897      455.3      391.2      14.076
0.7375      0.8870      435.3      374.2      14.046
0.7529      0.8841      414.1      355.9      14.053
0.7691      0.8810      391.6      336.2      14.157
0.7858      0.8778      366.8      315.2      14.060
0.8032      0.8744      340.6      292.8      14.031
0.8214      0.8708      312.7      268.7      14.067
0.8404      0.8670      282.5      242.9      14.030
0.8601      0.8630      250.2      215.3      13.934
0.881[illegible]      0.8588      215.2      185.3      13.875
0.9029      0.8542      177.4      153.1      13.721
0.9255      0.8495      137.8      118.9      13.748
0.9495      0.8444       94.5       81.6      13.683
0.9743      0.8390       48.7       42.0      13.699

RMS DEVIATION =    12.1033
```