ABSTRACT

Total vapor pressures of the binary mixtures cyclohexane-benzene, n-hexane-cyclohexane and n-hexane-benzene were determined by a static method over the temperature range from 0° to 25°C. The Antoine equation was used for the interpolation of the experimental data to 0°, 5°, 10°, 15°, 20° and 25°C. At these isothermal conditions, both direct and indirect methods were employed to calculate the vapor compositions and the total vapor pressures and it was shown that the results are in a close agreement, the standard deviation is less than 0.006 mole fraction and 0.3 mm Hg respectively.

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TABLE OF CONTENTS

CHAPTER		PAGE
	ABSTRACT	i
	ACKNOWLEDGEMENT	ii
	TABLE OF CONTENTS	iii
	LIST OF FIGURES	v
	LIST OF TABLES	vii
I	INTRODUCTION	1
II	LITERATURE SURVEY	3
	A. Experimental Determination of Vapor-Liquid Equilibrium	3
	B. Calculation Methods for Obtaining Equilibrium Vapor Compositions From Total Vapor Pressure-Liquid Composition Measurements	4
III	THEORETICAL CONSIDERATIONS	5
	A. Evaluation of Liquid Activity Coefficients and Vapor Compositions by the Indirect Method	5
	B. Evaluation of the Vapor Compositions by the Direct Method	10
IV	EXPERIMENTAL DETAILS	13
	A. Materials	13
	B. Apparatus	13
	1. Equilibrium Cell and the Solution reservoir	13
	2. Accessory Equipment used in connection with the Equilibrium Cell	15
	3. Equipment for Measuring the Physical Properties	16

CHAPTER		PAGE
	C. Experimental Procedure.....	16
	1. Test of the Apparatus by the Determination of Vapor Pressure of Pure Compounds and Mixtures.	16
	2. Determination of Total Vapor Pressures for Binary Mixtures...	17
	a) Preparation of Binary Liquid Mixtures	17
	b) Determination of Total Vapor Pressure as a Function of Temperature	17
	c) Analysis of Mixtures	18
V	RESULTS.....	19
VI	DISCUSSION.....	42
VII	CONCLUSION.....	56
VIII	NOMENCLATURE.....	57
IX	REFERENCES.....	58
X	APPENDIX.....	61

LIST OF FIGURES

FIGURE		PAGE
1	Schematic Diagram of the Apparatus	14
2	Total Vapor Pressure-Composition Diagram for the Cyclohexane - Benzene System	32
3	Vapor - Liquid Composition Diagram for the Cyclohexane - Benzene System	33
4	Liquid Activity Coefficient-Composition Diagram for the Cyclohexane - Benzene System	34
5	Total Vapor Pressure-Composition Diagram for the n-Hexane - Cyclohexane System.....	35
6	Vapor - Liquid Composition Diagram for the n-Hexane - Cyclohexane System.....	36
7	Liquid Activity Coefficients-Composition Diagram for n -Hexane - Cyclohexane System.....	37
8	Total Vapor Pressure-Composition Diagram for the n-Hexane - Benzene System.....	38
9	Liquid - Vapor Composition Diagram for the n-Hexane - Benzene System	39
10	Liquid Activity Coefficients-Composition Diagram for the n-Hexane - Benzene System	40
11	Excess Gibbs Free Energies at 25° C for the three binary systems	41

FIGURE		PAGE
12	Comparison of the Interpolated Total Vapor Pressure Values with Literature Data for the System Cyclohexane - Benzene at 10°C	44
13	Comparison of the Interpolated Total Vapor Pressure Values with Literature Data for the System n-Hexane - Benzene at 25°C	45
14	Comparison of the Extrapolated Total Vapor Pressure Values with Literature Data for the System Cyclohexane-Benzene at 39.99° and 69.98°C	50
15	Comparison of the Extrapolated Total Vapor Pressure Values with Literature Data for the System n-Hexane - Cyclohexane at 70°C.....	51
16	Comparison of the Extrapolated Total Vapor Pressure Values with Literature Data for the System n-Hexane - Benzene at 30°, 40°, 50° and 60°C	52
17	Comparison of the Extrapolated Bubble - Point Temperature Values with Literature Data for the System Cyclohexane-Benzene at 759 and 760 mm Hg.	53
18	Comparison of the Extrapolated Bubble-Point Temperature Values with Literature Data for the System n-Hexane - Cyclohexane at 760 mm Hg	54
19	Comparison of the Extrapolated Bubble-Point Temperature Values with Literature Data for the System n-Hexane - Benzene at 760 mm Hg.....	55

LIST OF TABLES

TABLE		PAGE
1	Physical Properties of the Materials Used	13
2	Total Vapor Pressure-Liquid Composition Data for the Cyclohexane-Benzene System	20
3	Total Vapor Pressures-Liquid Composition data for the n-Hexane-Cyclohexane System	21
4	Total Vapor Pressures-Liquid Composition data for the n-Hexane-Benzene System	22
5	Antoine Equation Constants Evaluated over the Temperature Range from 0° to 25° C	23
6	Redlich-Kister Constants for Correlating Liquid Activity Coefficients Obtained from the Indirect Method, and the Deviations Obtained from the Correlation	24
7	Constants for Correlating Total Vapor Pressures as a Function of Liquid Composition over the Temperature Range from 0° to 25° C.....	25
8	Comparison of the Calculated Results from the Direct and the Indirect Methods for the Cyclohexane-Benzene System	26
9	Comparison of the Calculated Results from the Direct and the Indirect Methods for the n-Hexane-Cyclohexane System.....	28

TABLE		PAGE
10	Comparison of the Calculated Results from the Direct and the Indirect Methods for the n-Hexane- Benzene System	30
11	Correlation of Total Vapor Pressure Data at Constant Liquid Compositions by Means of the Antoine Equation over the Temperature Range from 0°to 80°C	47
12	Comparison of Calculated Total Vapor Pressures from the Antoine Equation Constants of Table 11 with Literature Values	48
13	Constants for Correlation total vapor pressures as a function of Liquid Composition over a Temperature Range from 0° to 70°C.....	49

CHAPTER I

INTRODUCTION

Vapor - liquid equilibrium data for aromatic - saturated hydrocarbon mixtures are of interest to petroleum and petrochemical industries. The separation of the petroleum components is one of the most important operation processes in the chemical industry. Such mixtures are non-ideal and many mixtures of this type contain azeotropes. For efficient design of separation equipment, departures from ideal behaviour must be taken into account and reliable experimental data for the thermodynamic properties of mixtures are essential.

The purpose of this investigation was to determine the total vapor pressures for the binary systems cyclohexane-benzene, n-hexane-cyclohexane and n-hexane-benzene. These three binary systems were selected because they are the simplest representatives of the petroleum systems, containing combinations of an aromatic, a cycloparaffin and a straight-chain aliphatic hydrocarbon.

The vapor-liquid equilibrium data available in the literature for the three binary systems are listed in the following table:

System	Conditions	Reference
Cyclohexane-benzene	Isothermal at 39.99°C, 69.98°C	1
	10.0°C	6
	Isobaric at 760 mm Hg	2, 3
	759 mm Hg	4
n-hexane-cyclohexane	Isothermal at 70°C	5
	Isobaric at 760 mm Hg	2

n-hexane-benzene	Isothermal at 30°, 40°, 50°, 60°C	8
	25°C	9
	Isobaric at 760 mm Hg	2, 7, 10

For the systematic exploration of the field of vapor-liquid equilibrium, isothermal measurements are far more valuable than isobaric measurements. As observed from the above table, very few experimental data are available at the isothermal conditions, especially over the temperature range from 0° to 25°C.

The objectives of this study were to correlate the Antoine equation. This correlation, together with other thermodynamic relationships could then be used to compute equilibrium vapor compositions.

CHAPTER II

LITERATURE SURVEY

A. Experimental Determination of Vapor-Liquid Equilibrium

There are a large number of industrially important systems whose equilibrium relations cannot be predicted from purely theoretical considerations and which must be obtained by a direct experimental determination. The methods for the direct determination of equilibrium data can be generally classified into dynamic and static methods.

1) Dynamic Method [11,12,13,14]

The most typical example of this method is the circulation method. The vapor is circulated through a system and brought it back into repeated contact with the liquid until no further change in the composition of either phases can be detected. This method is usually done in an equilibrium still such as Othmer [11], Gillespie [12], Jones, Schoenborn and Colburn [13] and Ellis [14]. In such a dynamic method, the main disadvantage is in the difficulty in obtaining the true samples and their correct compositions at equilibrium conditions.

2) Static Method [15]

In this method, the equilibrium total vapor pressure of a degassed liquid mixture of known liquid composition is measured at isothermal conditions. This method has the advantage that the procedures for sampling and chemical analysis of the vapor composition can be avoided and the true equilibrium conditions can be assured.

B. Calculation Methods for Obtaining Equilibrium Vapor Compositions from Total Vapor Pressure-Liquid Composition Measurements

Over a period of years, considerable effort has been performed on the development and refinement of the methods of the direct measurements of pressures, temperatures and compositions of equilibrated vapor and liquid phases. Since it is difficult to determine the composition of the vapor phase at low pressure conditions, methods have been developed to predict the vapor composition from the properties of the liquid phase. The required data are the total vapor pressure, temperature and liquid phase composition. There are two approaches to the problem. One is the so called "indirect method" [16, 17, 18 - 24] in which, prior to the calculation, the equation representing concentration dependence of both liquid phase activity coefficients, must be chosen in such a way that the Gibbs-Duhem equation is fulfilled. Vapor phase compositions are then calculated from the activity coefficients. The other method is the direct calculation of vapor compositions [25, 26, 27] by an integration of the vapor-liquid coexisting equation. In this case, no prior assumption about the concentration dependence of the activity coefficients has to be assumed. However, some difficulties also arise because of the numerical integration involved. In this investigation, both "direct" and "indirect" methods were used to evaluate the vapor compositions and the results were compared.

CHAPTER III

THEORETICAL CONSIDERATIONS

At each constant composition, the temperature dependence of the vapor pressures of cyclohexane-benzene, n-hexane-cyclohexane and n-hexane-benzene systems in equilibrium with the liquid phase can be correlated by means of the Antoine equation

$$\log P = a - \frac{b}{t + c} \tag{1}$$

The calculated constants of the equation then can be used to obtain the relationship between the isothermal total vapor pressure and liquid composition.

A. Indirect Method

At low pressure conditions, assumptions can be made about the behavior of the vapor phase, in simplifying the deriving equations required for the calculation of liquid-phase activity coefficients from phase-equilibrium data. The activity coefficient is related to composition and is a precisely defined thermodynamic function,

$$\gamma_i = \frac{\hat{f}_i}{x_i f_i^o} \tag{2}$$

The condition of equilibrium requires that

$$\hat{f}_i^L = \hat{f}_i^V \tag{3}$$

$$\gamma_i^L x_i (f_i^o)^L = \gamma_i^V y_i (f_i^o)^V$$

$$\text{or} \qquad \gamma_i^{L} = \frac{y_i}{x_i} \frac{(f_i^{o})^{V}}{(f_i^{o})^{L}} \qquad \gamma_i^{V} = \frac{y_i}{x_i} \frac{(f_i^{o})^{V}/P}{(f_i^{o})^{L}/P} \qquad \gamma_i^{V} \qquad (4)$$

$$\text{or} \qquad \ln \gamma_i^{L} = \ln \frac{y_i}{x_i} + \ln \frac{\varphi_i^{V}}{\varphi_i^{L}} + \ln \gamma_i^{V} \qquad (5)$$

where

$\hat{f}_i$ = fugacity of component i in the solution

f_i^{o} = fugacity of pure component i at the standard state (i. e. at the temperature and pressure of the solution)

γ_i = activity coefficient of component i in the solution

φ_i = fugacity coefficient of pure component i

and the superscripts L and V denote the liquid and vapor phases respectively. At low pressures, the virial equation truncated after the second term is adequate for representing the vapor phase. Hence,

$$\ln \varphi_i^{V} = \frac{\beta_{ii} P}{R T} \qquad (6)$$

The liquid-phase $\ln \varphi_i^{L}$ must be calculated in two parts. At temperature T and at the vapor pressure of pure i, the fugacity coefficient for the liquid phase is equal to the fugacity coefficient of the vapor phase and is therefore given by the same equation:

$$\ln \varphi_i' = \frac{\beta_{ii} P_i}{R T} \qquad (7)$$

(') indicates values at the vapor pressure. Now the change in $\ln \varphi_i^{L}$ in going from the vapor pressure p_i to the solution pressure P is given by:

$$\ln \varphi_i^{L} - \ln \varphi_i' = \int_{p_i}^{P} \frac{-a_i}{R T} \, dP = \frac{1}{R T} \int_{p_i}^{P} \left(V_i^{L} - \frac{R T}{P} \right) dP \ldots\ldots \qquad (8)$$

or

$$\ln \varphi_i^L = \frac{\beta_{ii} p_i}{RT} + \frac{1}{RT} \int_{p_i}^{P} V_i^L \, dP - \ln \frac{P}{p_i} \qquad (9)$$

Since the volumes of liquids are insensitive to small changes in pressure, V_i^L may be taken as constant in the integral, giving

$$\ln \varphi_i^L = \frac{\beta_{ii} p_i}{RT} + \frac{V_i^L}{RT} (P - p_i) - \ln \frac{P}{p_i} \qquad (10)$$

combining the equations for $\ln \varphi_i^V$ and $\ln \varphi_i^L$ gives

$$\ln \frac{\varphi_i^V}{\varphi_i^L} = \frac{(\beta_{ii} - V_i^L)(P - p_i)}{RT} + \ln \frac{P}{p_i} \qquad (11)$$

Substituting Eq (11) in Eq (5), the following equation is obtained

$$\ln \gamma_i^L = \ln \frac{y_i P}{x_i p_i} + \frac{(\beta_{ii} - V_i^L)(P - p_i)}{RT} + \ln \gamma_i^V \qquad (12)$$

But

$$\ln \gamma_i^V = \frac{P \delta_{12} y_j^2}{RT} \qquad (13)$$

Thus for a binary solution at low pressures:

$$\ln \gamma_i^L = \ln \frac{y_i P}{x_i p_i} + \frac{(\beta_{ii} - V_i^L)(P - p_i)}{RT} + \frac{P \delta_{12} y_j^2}{RT} \qquad (14)$$

where

$$\delta_{12} = 2\beta_{12} - \beta_{11} - \beta_{22} \qquad (15)$$

Therefore

$$P = x_1 \gamma_1 p_1 \exp\left[\frac{-(\beta_{11} - V_1^L)(P - p_1) - P\delta_{12} y_2^2}{RT}\right] + x_2 \gamma_2 p_2 \exp\left[\frac{-(\beta_{22} - V_2^L)(P - p_2) - P\delta_{12} y_1^2}{RT}\right] \qquad (16)$$

The activity coefficients may be represented by means of an equation such as the Redlich-Kister[16].

$$\ln \gamma_1 = x_2^2 \left[B + C (4x_1 - 1) + D (2x_1 - 1) (6x_1 - 1) + \ldots \right] \quad (17a)$$

$$\ln \gamma_2 = x_1^2 \left[B + C (4x_1 - 3) + D(2x_1 - 1) (6x_1 - 5) + \ldots \right] \quad (17b)$$

In this investigation, the parameters of Eq (17) were evaluated by means of the non-linear regression technique proposed previously by Ho et al [17]. After substituting Eq (17) into Eq (16) the total vapor pressure in the new equation obtained is a function of liquid composition and coefficients B, C, D. This equation is used for the evaluation of B, C and D. Since it is non-linear with regard to the coefficients B, C and D, the following procedure was employed for their evaluation. A set of initial values of B, C and D was assigned using constants of a similar system as a guide. Using the first approximation the pressure residues, ΔP, and the derivatives $\partial P/\partial B$, $\partial P/\partial C$ and $\partial P/\partial D$ were determined by means of the following equations

$$\Delta P = P_{obs} - P_{calc} = \Delta B \frac{\partial P}{\partial B} + \Delta C \frac{\partial P}{\partial C} + \Delta D \frac{\partial P}{\partial D} \quad (18)$$

$$\frac{\partial P}{\partial B} = \left[x_1 (1 - x_1)^2 p_1 \gamma_1 + x_1^2 (1 - x_1) p_2 \gamma_2 \right] \quad (19a)$$

$$\frac{\partial P}{\partial C} = \left[x_1 (1 - x_1)^2 (4x_1 - 1) p_1 \gamma_1 + x_1^2 (1 - x_1) * (4x_1 - 3) p_2 \gamma_2 \right] \quad (19b)$$

$$\frac{\partial P}{\partial D} = \left[x_1 (1 - x_1)^2 (2x_1 - 1) (6x_1 - 1) p_1 \gamma_1 + x_1^2 (1 - x_1) * (2x_1 - 1) * (6x - 5) p_2 \gamma_2 \right] \quad (19c)$$

In obtaining Eq (19), the vapor phase was considered as an ideal gas. The calculation procedure is to determine the changes ΔB, ΔC, and ΔD in B, C and D so that the pressure residuals can be reduced to a minimum by means of the least-squares method, which is briefly described as follows. These increments are added to the initial values

of B, C and D for improved approximations. Thus, the quantities B, C and D are determined by successive approximations. The process is repeated until the increments ΔB, ΔC and ΔD are equal to or less than the tolerance desired in the values of B, C and D.

For "n" number of observations, there are "n" residual equations:

$$\Delta B \left(\frac{\partial P_1}{\partial B}\right) + \Delta C \left(\frac{\partial P_1}{\partial C}\right) + \Delta D \left(\frac{\partial P_1}{\partial D}\right) = \Delta P_1 \qquad (20)$$

$$\Delta B \left(\frac{\partial P_n}{\partial B}\right) + \Delta C \left(\frac{\partial P_n}{\partial C}\right) + \Delta D \left(\frac{\partial P_n}{\partial D}\right) = \Delta P_n$$

Therefore, the normal equations are

$$\Delta B \Sigma \left(\frac{\partial P}{\partial B}\right)^2 + \Delta C \Sigma \left(\frac{\partial P}{\partial B}\right)\left(\frac{\partial P}{\partial C}\right) + \Delta D \Sigma \left(\frac{\partial P}{\partial B}\right)\left(\frac{\partial P}{\partial D}\right) = \Sigma \Delta P \left(\frac{\partial P}{\partial B}\right)$$

$$\Delta B \Sigma \left(\frac{\partial P}{\partial B}\right)\left(\frac{\partial P}{\partial C}\right) + \Delta C \Sigma \left(\frac{\partial P}{\partial C}\right)^2 + \Delta D \Sigma \left(\frac{\partial P}{\partial C}\right)\left(\frac{\partial P}{\partial D}\right) = \Sigma \Delta P \left(\frac{\partial P}{\partial C}\right) \qquad (21)$$

and

$$\Delta B \Sigma \left(\frac{\partial P}{\partial B}\right)\left(\frac{\partial P}{\partial D}\right) + \Delta C \Sigma \left(\frac{\partial P}{\partial C}\right)\left(\frac{\partial P}{\partial D}\right) + \Delta D \Sigma \left(\frac{\partial P}{\partial D}\right)^2 = \Sigma \Delta P \left(\frac{\partial P}{\partial D}\right)$$

where the summations are taken over "n" observations. There are three normal equations as there are three unknowns B, C and D to be determined.

The second virial coefficients β_{11} and β_{22} may be calculated according to the equation of Pitzer and Curl [28].

$$\frac{p_{ci}\,\beta_{ii}}{R\,T_{ci}} = f\beta^{(0)}(TR) + \omega_i\, f\beta^{(1)}(TR) \qquad (22)$$

where p_{ci} = critical pressure of component i

T_{ci} = critical temperature of component i

ω_i = acentric factor of component i

$= -\log_{10}(p_i^s/p_{ci}) - 1.000$

p_i^s = saturated vapor pressure of i at $T/T_{ci} = 0.7$

$f\beta^{(0)}(TR)$ and $f\beta^{(1)}(TR)$ are the empirically determined functions

The cross coefficient β_{12} may be calculated according to the method by O'Connell and Prausnitz [29], in which Eq (22) is used with mixing rules for the various parameters.

In the actual calculation the third term on the right hand side of Eq (14) was neglected in the first approximation. The y values obtained from this approximation was used in the evaluation of this term in the second approximation. The calculation was repeated until the difference is within the precision required. The total vapor pressure, the vapor compositions, natural logarithm of liquid activity coefficients and the excess Gibbs free energies were then calculated. The excess Gibbs free energies are obtained from:

$$G^E = RT(x_1 \ln \gamma_1 + x_2 \ln \gamma_2) \qquad (23)$$

B. Direct Method

The method used in this investigation follows the modified procedure as described by Chang and Lu [26]. At moderately low pressures, the virial equation of state truncated to the second term, gives good

representation of the volumetric properties of vapor mixtures. Under these conditions, the equation for the direct evaluation of equilibrium vapor compositions for binary systems at constant temperature is given by

$$\frac{d\,y_1}{dP} = \frac{\psi - (1 - 2y_1)(y_1 - x_1)\,(\delta_{12}/RT)}{[\,(y_1 - x_1)/y_1\,(1 - y_1)\,] - (y_1 - x_1)\,(2\,P\,\delta_{12}/RT)} \tag{24}$$

in which

$$\psi = \frac{y_1\,y_2\,\delta_{12} - V^L + x_1\,\beta_{11} + x_2\,\beta_{22}}{RT} + 1/P \tag{25}$$

Assuming that the vapor phase is an ideal solution

$$\delta_{12} = 0 \tag{26}$$

and that

$$V^L = x_1\,V_1^o + x_2\,V_2^o$$

Equation (24) reduces to

$$\frac{dy_1}{dP} = \frac{\psi\,y_1\,(1 - y_1)}{(y_1 - x_1)} \tag{27}$$

which can be rearranged to give

$$\frac{d\,y_1}{d\,x_1} = \frac{\psi\,y_1\,(1 - y_1)}{(y_1 - x_1)} \qquad \frac{dP}{dx_1} \tag{28}$$

Numerical integration of Eq. (28) may proceed either from $x_1 = 0$ to $x_1 = 1$ or from $x_1 = 1$ to $x_1 = 0$.

An approximation has been used for the initial step of the integration

$$\frac{d\,y_1}{d\,x_1} = \frac{\Delta\,y_1}{\Delta\,x_1} \tag{29}$$

If the integration starts at $x_1 = 0$, then

$$\Delta y_1 = (y_1)_{x_1 = h} - (y_1)_{x_1 = 0} = (y_1)_{x_1 = h} \qquad (30)$$

and h is the size of the integrated step. With this approximation, the y_1 values at the end of the initial step can be solved algebraically.

$$(y_1)_{x_1 = h} = \left[\frac{x_1 [\, 1 + (\, dP/d\, x_1)\, \psi \,]}{1 + x_1 (\, dP/d\, x_1)\, \psi} \right]_{x_1 = h} \qquad (31)$$

Similar expression can be derived for the first approximation in the case that the integration proceed from $x_1 = 1$. The subsequent points were integrated by using the Runge-Kutta method.

The total vapor pressure - liquid composition values were correlated by means of

$$P = p_1 x_1 + p_2 x_2 + x_1 x_2 [C_1 + C_2 (x_1 - x_2) + C_3 (x_1 - x_2)^2 + . .]$$

$$. . . \qquad (32)$$

The quantity (dP/dx_1) used in Eq (28) and (31) was then calculated by differentiation of Eq (32).

Equation (28) is not continuous in the azeotropic point where $dP/dx_1 = 0$ and $y_1 - x_1 = 0$. Therefore in the presence of an azeotrope, numerical integration should proceed from $x_1 = 0$ to x azeotrope and then from $x_1 = 1$ down to x azeotrope. Care should also be taken in the selection of how many coefficients will be used in Eq. (32) as the calculated P-x curve tends to "wobble" in some cases.

CHAPTER IV

EXPERIMENTAL DETAILS

A. Materials

Research grade n-hexane (99.99 mole % purity), cyclohexane (99.99 mole % purity) and benzene (99.90 mole % purity) supplied by Philips Petroleum Co. were used without further purification. The refractive indices and densities of the pure components measured are listed in Table 1.

TABLE 1

Physical Properties of the Materials Used at 25°C

Material	Expte	Lit	Reference
Refractive Index			
n-Hexane	1.37230	1.37226	2
Cyclohexane	1.42351	1.42354	2
Benzene	1.49787	1.49790	2
Density			
n-Hexane	0.65490	0.65480	2
Cyclohexane	0.77383	0.77389	2
Benzene	0.87384	0.87368	2

B. Apparatus

1. Equilibrium Cell and the Solution Reservoir

The arrangement of the apparatus is schematically shown in figure 1. The main parts of the apparatus consists of an equilibrium cell and a solution reservoir.

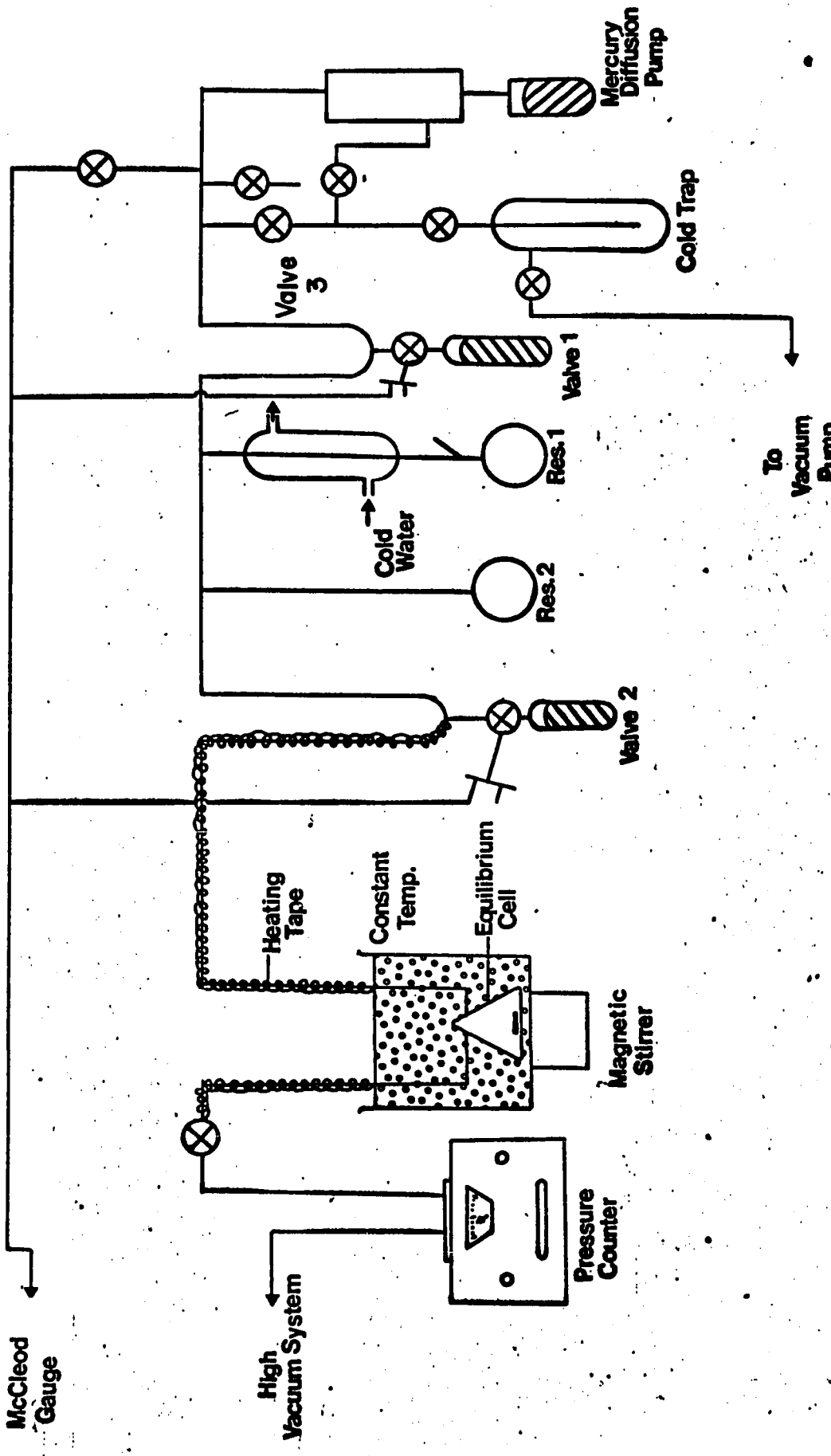

Fig. 1 - Schematic Diagram of the Apparatus

The equilibrium cell was made of a 100 ml flat-bottomed Pyrex flask containing a small magnetic stirrer. The cell was connected to a precision quartz gauge (Texas Instruments, Model 144-01, Serial Number 1981) which had been calibrated by measuring the total vapor pressures of the pure components: benzene, cyclohexane and n-hexane. The quartz spiral of the gauge was thermostated at 44.2 ± 0.1°C.

The solution reservoir is made of a 100 ml round-bottomed Pyrex flask which can be isolated from the system by means of two u-tube mercury seal-off valves (valve 1 and 2). These values could be by-passed to the vacuum manifold or to the atmosphere by a three way stop-cock so that the mercury level in the u-tube could be manipulated A capillary tube is connected to the upper part of the reservoir through which the liquid solution is introduced. A Liebig condenser was built above the reservoir to condense and reflux the vaporized materials from the reservoir.

2. Accessory Equipment Used in Connection with the Equilibrium Cell

They are divided into two parts:

(i) Temperature Measuring Device

Temperature was measured by means of a Leeds and Northrup K-3 potentiometer with a SRI Tinsley galvanometer using a 5-junction iron-constantan thermopile. The thermocouple was calibrated by comparison with a standard platinum resistance thermometer. The calibration is tabulated as shown in appendix I. For isothermal operations, the desired temperatures from 0° to 25°C were obtained and regulated by a thermotrol and a cooler.

(ii) Pressure Measurement Device

The pressure of the system was read from a precision quartz pressure gauge (Texas Instruments). The calibration table is shown in Appendix II.

3. Equipment for Physical Properties Measurements

(i) Refractometer

A Bausch and Lomb Abb-3L precision refractometer and sodium lamp were used to determine the refractive indices of the pure components. The prism temperature was kept constant at 25°C ± 0.02°C.

(ii) Pycnometer (for quantitative analysis)

Pycnometers were used to measure the densities of the mixtures at 25°C. The volume of the pycnometers were found by using distilled water. The density-liquid composition calibration table for the three binary systems are shown in Appendix III.

C. Experimental Procedure

1. Test of the Apparatus by the Determination of Total Vapor Pressure of Pure Compounds and Mixtures

The equipment was used previously by the author [8] to obtain the P-t-x data on the following pure compounds and mixtures:

(i) Benzene, n-hexane, toluene and n-pentane at a temperature range from 25°C to 60°C. They agree extremely well with the total vapor pressures calculated from the Antoine equation constants reported in the literature [30].

(ii) Total vapor pressures were measured for the system n-hexane-benzene from 30° to 60°C and for the system toluene-n-pentane from 20° to 40°C. The data are reliable by comparing with literature data.

The equipment was then improved by replacing the mercury manometer with a precision pressure gauge. More accurate total vapor pressure values could be obtained. The total vapor pressures of pure components benzene, n-hexane and cyclohexane were measured from 0°to 25°C. They agree very well with the vapor pressures calculated from the Antoine equation constants reported in the literature [1, 2].

2. Determination of Total Vapor Pressures for the Binary Systems

(a) Preparation of Binary Liquid Mixtures

A 100 ml volumetric flask containing a magnetic stirrer was first weighed. The less volatile component of the mixture was then added and the weight was obtained. The other component was subsequently added to fill up the flask to the 100 ml mark and weighed. The mixture, of known liquid composition, was mixed thoroughly by means of a magnetic stirrer.

(b) Experimental Procedure

The whole apparatus was evacuated. The valve 2 was closed in order to isolate the equilibrium cell and the pressure gage from the system. About 80 ml of the sample solution of known composition was introduced into the reservoir through the capillary tube with an hypodermic syringe. The reservoir was immersed in liquid nitrogen in a Dewar flask. After the liquid sample was cooled, the capillary was sealed off and the degassing procedure of the solution

followed. Valve 3 was opened and all the non-condensable gas was evacuated. Then valve 3 and valve 1 were closed and the reservoir was heated to expel the dissolved or trapped gases in the solution, which was then again cooled down and the non-condensable gas evacuated. The process was repeated until no change of the residual vacuum could be detected (0.0005 mm Hg).

When the whole apparatus was evacuated, valve 1 was closed and valve 2 was opened and the degassed solution was distilled into the equilibrium cell, which was then totally immersed into a constant temperature bath. After equilibrium was established, the total vapor pressure measurements were recorded from the pressure gauge. Precision of the temperature measurement is estimated to be ± 0.005°C, and of the pressure measurements, ± 0.03 mm Hg.

(c) Analysis of Mixtures

A sample of the solution was obtained and the liquid composition of the solution was determined by measuring its density at 25°C. Precision of the composition measurements is estimated to be ± 0.0005 mole fractions.

CHAPTER V

RESULTS

Experimental Data

Vapor pressure of the three binary systems containing n-hexane, cyclohexane and benzene were measured over the temperature range from 0°to 25°C, and are tabulated in Tables 2, 3 and 4.

Correlation of Results

At each constant composition, the total vapor pressures were correlated by the Antoine equation and the constants of the equation are listed in Table 5. Redlich-Kister constants are listed in Table 6. Constants for correlating total vapor pressures as a function of liquid composition over a temperature range from 0° to 25°C are listed in Table 7. Calculated results of Pcalc, y, γ and G^E for the three binary systems are listed in Tables 8, 9, and 10.

The graphical presentation of results for these three systems are shown in Figures 2 - 11.

TABLE 2

Total Vapor Pressure-Liquid Composition Data for the Cyclohexane-Benzene System

t°C	Pobs(mm Hg)	t°C	Pobs(mm Hg)	t°C	Pobs(mm Hg)	t°C	Pobs(mm Hg)
$x_1 = 0$		$x_1 = 0.102$		$x_1 = 0.174$		$x_1 = 0.418$	
6.68	38.16	0.50	29.83	0.45	31.40	0.53	32.92
7.02	38.94	2.51	33.36	3.24	36.45	6.13	44.13
9.88	45.30	6.30	40.63	5.77	41.66	10.23	54.36
10.07	45.70	10.18	49.81	9.35	50.06	14.19	66.20
11.43	49 18	13.59	59.09	12.58	58.89	17.74	78.51
12.80	52.71	16.91	69.57	17.04	73.16	21.68	94.37
13.47	54.49	20.87	83.99	21.08	88.66	25.06	109.93
15.29	59.60	25.51	104.07	24.94	105.61		
16.63	63.89						
17.97	68.13						
20.00	75.31						
20.07	75.54						
22.34	84.13						
25.05	95.59						
25.32	96.66						

t°C	Pobs(mm Hg)	t°C	Pobs(mm Hg)	t°C	Pobs(mm Hg)	t°C	Pobs(mm Hg)
$x_1 = 0.735$		$x_1 = 0.838$		$x_1 = 0.923$		$x_1 = 1.000$	
0.63	32.98	0.62	31.91	0.42	30.13	6.08	38.73
4.41	40.34	3.69	37.60	3.18	34.96	10.70	49.32
8.28	49.37	7.14	44.81	5.56	39.74	12.53	54.21
11.97	59.28	9.66	50.97	6.10	40.88	15.03	61.20
16.52	73.97	12.80	59.58	10.33	50.67	17.23	68.21
20.48	89.11	16.00	69.63	13.99	60.84	20.74	80.39
22.37	97.23	18.87	79.71	17.86	73.30	23.13	89.90
24.92	109.00	21.66	90.59	21.82	88.13	25.14	98.41
		25.00	105.03	25.05	102.11		

TABLE 3

Total Vapor Pressure-Liquid Composition Data for the n-Hexane-Cyclohexane System

t°C	Pobs (mm Hg)	t°C	Pobs (mm Hg)	t°C	Pobs (mm Hg)
x_1 = 0.064		x_1 = 0.321		x_1 = 0.349	
0.60	31.06	0.61	37.27	0.52	37.14
3.74	36.74	3.49	43.24	5.21	47.33
8.49	46.95	4.92	46.52	10.43	61.51
12.19	56.66	6.24	49.76	14.98	76.61
16.23	68.81	10.30	60.93	17.27	85.31
20.83	85.47	13.31	70.45	20.43	98.56
25.42	105.10	14.90	75.79	24.99	120.86
		17.98	87.46		
		21.41	101.98		

t°C	Pobs(mm Hg)	t°C	Pobs(mm Hg)	t°C	Pobs(mm Hg)	t°C	Pobs(mm Hg)
x_1 = 0.504		x_1 = 0.736		x_1 = 0.850		x_1 = 1.000	
0.48	40.46	0.37	42.80	0.57	44.81	0.43	46.41
4.35	49.51	3.41	50.15	4.18	54.04	1.64	49.48
8.26	60.31	8.32	64.24	7.93	65.39	3.53	54.68
12.43	73.98	12.53	79.04	13.06	84.25	5.65	60.77
15.77	86.60	16.53	95.63	16.13	97.13	8.05	68.79
19.46	102.69	20.67	115.52	20.51	118.82	9.93	75.43
25.02	131.63	24.93	139.52			12.56	85.77
						14.93	96.00
						17.53	108.44
						19.96	121.18
						22.33	134.56
						25.17	152.53

TABLE 4

Total Vapor Pressures-Liquid Composition Data for the n-Hexane-Benzene System

t°C	Pobs (mm Hg)	t°C	Pobs (mm Hg)	t°C	Pobs (mm Hg)
x_1 = 0.048		x_1 = 0.118		x_1 = 0.269	
5.28	40.07	0.47	34.80	0.53	39.98
10.42	52.43	3.74	41.29	3.95	47.91
14.98	65.66	6.61	47.94	7.34	57.02
17.98	75.91	10.74	59.13	10.77	67.21
21.07	87.97	16.22	77.12	16.57	89.12
24.98	105.13	21.14	96.96	20.25	105.54
		24.36	112.09	24.10	125.27

t°C	Pobs(mm Hg)	t°C	Pobs(mm Hg)	t°C	Pobs(mm Hg)	t°C	Pobs(mm Hg)
x_1 = 0.366		x_1 = 0.501		x_1 = 0.735		x_1 = 0.910	
0.70	42.61	1.17	45.88	0.84	47.39	0.38	46.99
4.15	50.93	5.11	56.22	5.33	59.74	4.77	58.99
7.63	61.08	9.29	69.43	10.48	77.23	8.69	71.84
12.83	78.66	13.56	85.44	13.91	90.96	13.85	92.14
16.55	93.64	17.24	101.27	17.68	108.52	17.95	111.47
20.15	110.59	20.81	119.18	21.15	126.83	20.71	126.30
25.06	137.38	24.91	142.98	25.30	152.25	25.16	153.65

TABLE 5

* Antoine Equation Constants Evaluated Over the Temperature Range from 0° to 25°C

x_1	a	b	c	dev. mm Hg	dev. Per cent
Cyclohexane-Benzene					
0.000	6.96343	1237.825	223.340	0.07	0.11
0.102	7.53637	1542.020	253.895	0.06	0.15
0.174	7.49495	1524.031	253.630	0.06	0.08
0.418	7.67334	1621.910	262.928	0.08	0.11
0.635	7.12865	1336.133	237.524	0.05	0.08
0.838	7.05846	1315.966	236.285	0.10	0.16
0.923	7.00396	1282.882	231.782	0.04	0.09
1.000	6.36153	981.989	199.645	0.07	0.11
n-Hexane-Cyclohexane					
0.000	6.36153	981.989	199.695	0.07	0.11
0.064	6.93232	1251.582	229.450	0.06	0.11
0.321	6.54830	1073.091	214.966	0.06	0.11
0.349	7.22000	1385.402	244.663	0.03	0.06
0.544	7.20582	1364.571	243.252	0.03	0.04
0.736	7.09476	1292.816	236.242	0.07	0.11
0.850	6.76029	1125.796	219.763	0.11	0.16
1.000	6.86222	1163.436	223.485	0.07	0.10
n-Hexane-Benzene					
0.000	6.96343	1237.825	223.340	0.07	0.11
0.048	6.96618	1247.376	227.301	0.08	0.13
0.118	7.06454	1300.516	234.969	0.05	0.13
0.269	6.98980	1252.119	231.859	0.15	0.24
0.366	6.79161	1150.587	222.180	0.11	0.17
0.501	6.97154	1230.136	230.494	0.09	0.10
0.735	6.99120	1233.325	231.178	0.05	0.05
0.910	7.07062	1269.972	234.861	0.02	0.03
1.000	6.86222	1163.436	223.485	0.07	0.10

* $\text{Log}_{10}\, p = a - \frac{b}{t + c}$

TABLE 6

Redlich-Kister Constants for Correlating Liquid Activity Coefficients Obtained from the Indirect Method, and the Deviations Obtained from the Correlation

t°C	B	C	D	St Dev mm Hg	Ave % Dev.
Cyclohexane-Benzene					
0	0.68153	-0.06759	0.13845	0.18	0.41
5	0.63873	-0.05811	0.12093	0.21	0.33
10	0.60295	-0.05241	0.10381	0.25	0.29
15	0.57340	-0.05074	0.08817	0.30	0.27
20	0.54945	-0.05269	0.07408	0.35	0.24
25	0.53045	-0.05819	0.06222	0.39	0.19
n-Hexane-Cyclohexane					
0	0.24752	-0.10364	0.01142	0.16	0.27
5	0.22211	-0.09483	0.01935	0.18	0.21
10	0.19985	-0.08396	0.02179	0.20	0.19
15	0.17993	-0.07093	0.02123	0.22	0.18
20	0.16256	-0.05683	0.01900	0.23	0.15
25	0.14729	-0.04020	0.01352	0.30	0.16
n-Hexane-Benzene					
0	0.76000	-0.10004	0.08646	0.10	0.14
5	0.72859	-0.10314	0.06985	0.12	0.14
10	0.69871	-0.10339	0.06011	0.15	0.15
15	0.67082	-0.10235	0.05265	0.19	0.14
20	0.64442	-0.09992	0.04786	0.23	0.14
25	0.61947	-0.09652	0.04754	0.27	0.14

TABLE 7

Constants for Correlating Total Vapor Pressures as a Function of Liquid Composition over the Temperature range from 0° to 25°C

t°C	C_1	C_2	C_3	C_4*	St Dev mm Hg	Dev %	Max x_1	Max P mm Hg
Cyclohexane-Benzene								
0	20.077	- 2.4438	12.385		0.16	0.53	.508	32.06
5	24.529	- 3.1636	13.477		0.21	0.54	.505	41.85
10	29.934	- 4.1094	14.598		0.27	0.54	.499	54.06
15	36.537	- 5.1365	15.875		0.34	0.52	.494	69.16
20	44.636	- 6.4458	17.515		0.40	0.49	.487	87.68
25	54.589	- 8.0325	19.936		0.45	0.43	.478	110.20
n-Hexane-Cyclohexane								
0	8.6651	- 6.6404	4.1282		0.21	0.59		
5	9.8748	- 7.2259	4.3775		0.24	0.52		
10	11.318	- 7.6564	4.1787		0.26	0.44		
15	13.000	- 7.9810	3.6377		0.27	0:35		
20	15.068	- 8.1215	2.7151		0.26	0.28		
25	18.078	- 2.9486	0.2351	-16.507	0.19	0.14		
n-Hexane-Benzene								
0	28.307	-13.632	19.082		0.19	0.55	.882	46.11
5	35.446	-17.136	22.068		0.23	0.52	.888	59.75
10	43.943	-21.002	25.636		0.29	0.50	.892	76.64
15	53.926	-25.378	29.563		0.34	0.47	.896	97.31
20	65.593	-30.157	34.016		0.40	0.43	.899	122.41
25	79.454	-30.970	38.035	-11.658	0.46	0.38	.901	152.62

* Constants from Equation (32)

TABLE 8

Comparison of the Calculated Results from the Direct and the Indirect Methods for the Cyclohexane-Benzene System

		Indirect Method					G^E	Direct Method	
T °C	Pobs mmHg	x_1	Pcalc mmHg	y_1	$\ln\gamma_1$	$\ln\gamma_2$	cal/gmole	Pcalc mmHg	y_1
0	26.37	0.000	26.36	0.000	0.8876	0.000	0.00		0.000
	29.05	0.102	29.27	0.179	0.6172	0.0138	40.90	29.24	0.182
	30.64	0.174	30.39	0.257	0.4763	0.0362	61.21	30.48	0.264
	31.99	0.418	32.03	0.446	0.2037	0.1448	91.96	32.00	0.436
	31.89	0.635	31.99	0.606	0.0910	0.2693	84.72	31.94	0.614
	30.85	0.838	30.71	0.778	0.0237	0.4633	51.52	30.77	0.773
	29.47	0.923	29.55	0.876	0.0061	0.5950	27.92	29.53	0.871
	27.72	1.000	27.86	1.000	0.000	0.7524	0.00		1.000
5	34.87	0.000	34.86	0.000	0.8178	0.000	0.00		0.000
	38.06	0.102	38.33	0.172	0.5737	0.0125	38.55	38.30	0.175
	40.04	0.174	39.72	0.250	0.4455	0.0328	57.82	39.81	0.256
	41.70	0.418	41.78	0.445	0.1928	0.1339	87.62	41.76	0.436
	41.65	0.635	41.73	0.607	0.0854	0.2526	80.93	41.66	0.613
	40.25	0.838	40.10	0.782	0.0219	0.4354	49.13	40.16	0.780
	38.57	0.923	38.66	0.879	0.0056	0.5573	26.58	38.67	0.877
	36.56	1.000	36.60	1.000	0.000	0.7015	0.00		1.000
10	45.66	0.000	45.56	0.000	0.7592	0.000	0.00		0.000
	49.36	0.102	49.69	0.166	0.5378	0.0114	36.62	49.66	0.169
	51.80	0.174	51.40	0.245	0.4202	0.0300	55.08	51.49	0.250
	53.83	0.418	53.96	0.443	0.1834	0.1251	84.10	53.95	0.436
	53.82	0.635	53.86	0.607	0.0801	0.2393	77.76	53.78	0.612
	51.94	0.838	51.80	0.784	0.0201	0.4115	46.98	51.85	0.784
	49.92	0.923	50.01	0.882	0.0051	0.5235	25.33	50.06	0.882
	47.59	1.000	47.52	1.000	0.000	0.6544	0.00		1.000

	Indirect Method						G^E cal	Direct Method	
°C	Pobs mmHg	x_1	Pcalc mmHg	y_1	$\ln\gamma_1$	$\ln\gamma_2$	g mole	Pcalc mmHg	y_1
15	58.87	0.000	58.87	0.000	0.7123	0.000	0.00		0.000
	63.39	0.102	63.79	0.162	0.5092	0.0105	35.14	63.75	0.164
	66.36	0.174	65.88	0.241	0.4000	0.0278	53.00	65.97	0.245
	68.86	0.418	69.03	0.441	0.1751	0.1184	81.36	69.03	0.435
	68.84	0.635	68.86	0.607	0.0749	0.2291	75.11	68.75	0.610
	66.35	0.838	66.24	0.787	0.0183	0.3910	45.05	66.28	0.788
	63.95	0.923	64.02	0.884	0.0046	0.4932	24.18	64.10	0.885
	61.18	1.000	61.03	1.000	0.000	0.6108	0.00		1.000
20	75.27	0.000	75.26	0.000	0.6762	0.000	0.00		0.000
	80.67	0.102	81.15	0.158	0.4873	0.0098	34.08	81.10	0.160
	84.26	0.174	83.70	0.237	0.3844	0.0261	51.52	83.79	0.241
	87.32	0.418	87.52	0.439	0.1677	0.1136	79.35	87.54	0.434
	87.22	0.635	87.21	0.606	0.0699	0.2217	72.99	87.09	0.609
	83.95	0.838	83.87	0.788	0.0165	0.3735	43.30	83.91	0.789
	81.11	0.923	81.15	0.887	0.0041	0.4661	23.11	81.24	0.887
	77.76	1.000	77.58	1.000	0.000	0.5708	0.00		1.000
25	95.29	0.000	95.26	0.000	0.6509	0.000	0.00		0.000
	101.79	0.102	102.34	0.155	0.4716	0.0093	33.45	102.29	0.157
	106.07	0.174	105.43	0.234	0.3728	0.0250	50.66	105.54	0.237
	109.82	0.418	110.03	0.437	0.1610	0.1108	78.07	110.06	0.432
	109.51	0.635	109.49	0.635	0.6051	0.2166	71.33	109.36	0.607
	105.27	0.838	105.24	0.790	0.0148	0.3587	41.77	105.29	0.790
	101.93	0.923	101.91	0.888	0.0036	0.4421	22.14	102.00	0.888
	97.78	1.000	97.66	1.000	0.000	0.5345	0.00		1.000

TABLE 9

Comparison of the Calculated Results from the Direct and the Indirect Methods for the n-Hexane - Cyclohexane System

T	Indirect Method							Direct Method	
°C	Pobs mmHg	x_1	Pcalc mmHg	y_1	$\ln\gamma_1$	$\ln\gamma_2$	G^E cal/gmole	Pcalc mmHg	y_1
0	27.72	0.000	27.86	0.000	0.3626	0.000	0.00		0.000
	30.03	0.064	30.01	0.129	0.2900	0.0024	11.29	29.90	0.130
	36.01	0.321	35.85	0.447	0.0989	0.0451	33.85	35.89	0.450
	36.10	0.349	36.34	0.474	0.0858	0.0517	34.52	36.37	0.476
	39.46	0.544	39.34	0.643	0.0266	0.0980	32.11	39.31	0.642
	41.91	0.736	41.94	0.799	0.0045	0.1355	21.21	41.93	0.800
	43.40	0.850	43.43	0.888	0.0007	0.1495	12.50	43.45	0.889
	45.32	1.000	45.34	1.000	0.000	0.1553	0.00		1.000
5	36.56	0.000	36.60	0.000	0.3363	0.000	0.00		0.000
	39.26	0.064	39.24	0.125	0.2657	0.0023	10.59	39.16	0.124
	46.76	0.321	46.54	0.442	0.0872	0.0418	31.16	46.58	0.444
	46.87	0.349	47.17	0.470	0.0754	0.0477	31.71	47.19	0.471
	51.18	0.544	51.05	0.642	0.0238	0.0880	29.34	51.02	0.641
	54.42	0.736	54.48	0.800	0.0048	0.1203	19.51	54.46	0.800
	56.43	0.850	56.43	0.889	0.0011	0.1341	11.63	56.45	0.889
	58.92	1.000	58.93	1.000	0.000	0.1466	0.00		1.000
10	47.59	0.000	47.52	0.000	0.3056	0.000	0.00		0.000
	50.75	0.064	50.73	0.121	0.2403	0.0021	9.759	50.66	0.119
	60.02	0.321	59.78	0.438	0.0779	0.0379	28.55	59.80	0.440
	60.24	0.349	60.58	0.466	0.0675	0.0431	29.04	60.59	0.467
	65.71	0.544	65.55	0.642	0.0219	0.0786	26.87	65.55	0.641
	69.92	0.736	69.99	0.800	0.0050	0.1076	18.05	69.98	0.800
	72.52	0.850	72.52	0.889	0.0014	0.1212	10.91	72.53	0.889
	75.73	1.000	75.74	1.000	0.000	0.1377	0.00		1.000

	Indirect Method					Direct Method			
T °C	Pobs mmHg	x_1	Pcacl mmHg	y_1	$\ln\gamma_1$	$\ln\gamma_2$	$\frac{G^E_{cal}}{g\,mole}$	Pcalc mmHg	y_1
15	61.18	0.000	61.03	0.000	0.2721	0.000	0.00		0.000
	64.91	0.064	64.85	0.117	0.2140	0.0019	8.860	64.79	0.115
	76.21	0.321	76.01	0.435	0.0705	0.0334	25.94	76.02	0.437
	76.67	0.349	77.02	0.463	0.0613	0.0381	26.51	77.02	0.465
	83.55	0.544	83.34	0.641	0.0210	0.0696	24.71	83.36	0.641
	88.93	0.736	89.02	0.800	0.0053	0.0965	16.82	89.00	0.800
	92.22	0.850	92.25	0.889	0.0016	0.1106	10.28	92.23	0.889
	96.33	1.000	96.33	1.000	0.000	0.1302	0.00		1.000
20	77.76	0.000	77.58	0.000	0.2384	0.000	0.00		0.000
	82.22	0.064	82.08	0.113	0.1885	0.0016	7.900	82.00	0.111
	95.79	0.321	95.73	0.432	0.0647	0.0289	23.53	95.74	0.434
	96.70	0.349	97.00	0.461	0.0566	0.0330	24.02	97.00	0.463
	105.27	0.544	104.97	0.641	0.2007	0.0611	24.54	105.02	0.641
	112.06	0.736	112.14	0.800	0.0058	0.0869	15.85	112.12	0.800
	116.10	0.850	116.20	0.889	0.0018	0.1020	9.80	116.15	0.889
	121.32	1.000	121.32	1.000	0.000	0.1247	0.00		1.000
25	97.78	0.000	97.66	0.000	0.2010	0.000	0.00		0.000
	103.17	0.064	102.89	0.110	0.1617	0.0013	6.85	103.11	0.110
	119.25	0.321	119.49	0.430	0.0607	0.0238	21.12	119.33	0.429
	120.91	0.349	121.07	0.459	0.0537	0.0273	21.63	120.91	0.458
	131.50	0.544	131.05	0.641	0.0214	0.0528	21.16	131.36	0.644
	139.97	0.736	140.01	0.800	0.0063	0.0790	15.10	140.15	0.798
	144.80	0.850	145.06	0.889	0.0020	0.0955	9.49	144.68	0.885
	151.39	1.000	151.39	1.000	0.000	0.1206	0.00		1.000

TABLE 10

Comparison of the Calculated Results from the Direct and the Indirect Methods for n-Hexane-Benzene System

T °C	Pobs mmHg	x_1	Indirect Method Pcalc mmHg	y_1	$\ln\gamma_1$	$\ln\gamma_2$	G^E cal/g mole	Direct Method Pcalc mmHg	y_1
0	26.37	0.000	26.36	0.000	0.9465	0.000	0.00		0.000
	30.09	0.048	30.06	0.162	0.8133	0.0032	22.84	29.85	0.157
	33.86	0.118	33.90	0.301	0.6471	0.0181	50.11	33.80	0.302
	38.85	0.269	38.85	0.463	0.3891	0.0787	88.04	39.07	0.470
	41.02	0.366	40.95	0.534	0.2752	0.1314	99.89	41.04	0.535
	43.11	0.501	43.11	0.620	0.1646	0.2154	103.10	42.93	0.613
	45.32	0.735	45.47	0.770	0.0496	0.4005	77.39	45.38	0.777
	46.06	0.910	45.89	0.905	0.0066	0.6033	32.73	46.07	0.904
	45.32	1.000	45.34	1.000	0.000	0.7464	0.00		1.000
5	34.87	0.000	34.87	0.000	0.9016	0.000	0.00		0.000
	39.49	0.048	39.42	0.155	0.7773	0.0030	22.20	39.18	0.151
	44.16	0.118	44.23	0.292	0.6211	0.0170	58.80	44.10	0.293
	50.52	0.269	50.55	0.455	0.3747	0.0749	85.97	50.79	0.462
	53.33	0.366	53.22	0.528	0.2641	0.1261	97.61	53.33	0.529
	55.96	0.501	55.96	0.616	0.1560	0.2083	100.65	55.77	0.609
	58.77	0.735	58.94	0.768	0.0451	0.3861	74.87	58.83	0.775
	59.70	0.910	59.51	0.906	0.0058	0.5705	31.30	59.72	0.906
	58.92	1.000	58.93	1.000	0.000	0.6953	0.00		1.000
10	45.56	0.000	45.56	0.000	0.8622	0.000	0.00		0.000
	51.25	0.048	51.12	0.148	0.7447	0.0028	21.61	50.84	0.145
	56.97	0.118	57.07	0.284	0.5963	0.0161	47.60	56.92	0.285
	64.97	0.269	65.02	0.448	0.3602	0.0717	84.01	65.30	0.455
	68.55	0.366	68.39	0.522	0.2534	0.1212	95.42	68.53	0.524
	71.86	0.501	71.86	0.612	0.1484	0.2009	98.24	71.65	0.606
	75.41	0.735	75.61	0.767	0.0419	0.3715	72.72	75.47	0.773
	76.58	0.910	76.37	0.907	0.0052	0.5426	30.14	76.61	0.907
	75.73	1.000	75.74	1.000	0.000	0.6554	0.00		1.000

		Indirect Method						Direct Method	
T °C	Pobs mmHg	x_1	Pcalc mmHg	y_1	$\ln\gamma_i$	$\ln\gamma_2$	G^E $\frac{cal}{g\,mole}$	Pcalc mmHg	y_1
15	58.87	0.000	58.87	0.000	0.8258	0.000	0.00		0.000
	65.79	0.048	65.60	0.143	0.7143	0.0027	21.10	65.28	0.139
	72.75	0.118	72.91	0.276	0.5728	0.0154	46.48	72.72	0.277
	82.72	0.269	82.78	0.442	0.3464	0.0687	82.11	83.10	0.448
	87.19	0.366	87.00	0.517	0.2433	0.1165	93.28	87.16	0.518
	91.34	0.501	91.33	0.608	0.1417	0.1937	95.99	91.11	0.603
	95.79	0.735	96.02	0.766	0.0392	0.3575	70.74	95.86	0.771
	97.25	0.910	97.02	0.908	0.0048	0.5177	29.18	97.30	0.908
	96.33	1.000	96.33	1.000	0.000	0.6211	0.00		1.000
20	75.27	0.000	75.26	0.000	0.7922	0.000	0.00		0.000
	83.60	0.048	83.35	0.137	0.6858	0.0026	20.62	82.99	0.134
	92.01	0.118	92.23	0.269	0.5505	0.0147	45.39	91.99	0.269
	104.30	0.269	104.37	0.435	0.3332	0.0659	80.27	104.72	0.441
	109.81	0.366	109.60	0.512	0.2338	0.1120	91.21	109.79	0.513
	115.00	0.501	114.97	0.605	0.1358	0.1864	93.81	114.72	0.600
	120.51	0.735	120.51	0.766	0.0371	0.3439	68.97	120.60	0.770
	122.35	0.910	122.08	0.909	0.0045	0.4956	28.37	122.40	0.909
	121.32	1.000	121.32	1.000	0.000	0.5924	0.00		1.000
25	95.29	0.000	95.26	0.000	0.7635	0.000	0.00		0.000
	105.24	0.048	104.93	0.133	0.6605	0.0025	20.19	104.71	0.128
	115.33	0.118	115.61	0.262	0.5296	0.0142	44.44	115.49	0.260
	130.33	0.269	130.38	0.429	0.3200	0.0636	78.54	130.64	0.434
	137.01	0.366	136.80	0.507	0.2244	0.1079	89.19	136.87	0.509
	143.48	0.501	143.42	0.601	0.1304	0.1793	91.71	143.24	0.601
	150.27	0.735	150.60	0.765	0.0358	0.3304	67.46	150.56	0.771
	152.58	0.910	152.26	0.909	0.0044	0.4767	27.79	152.34	0.908
	151.39	1.000	151.39	1.000	0.000	0.5705	0.00		1.000

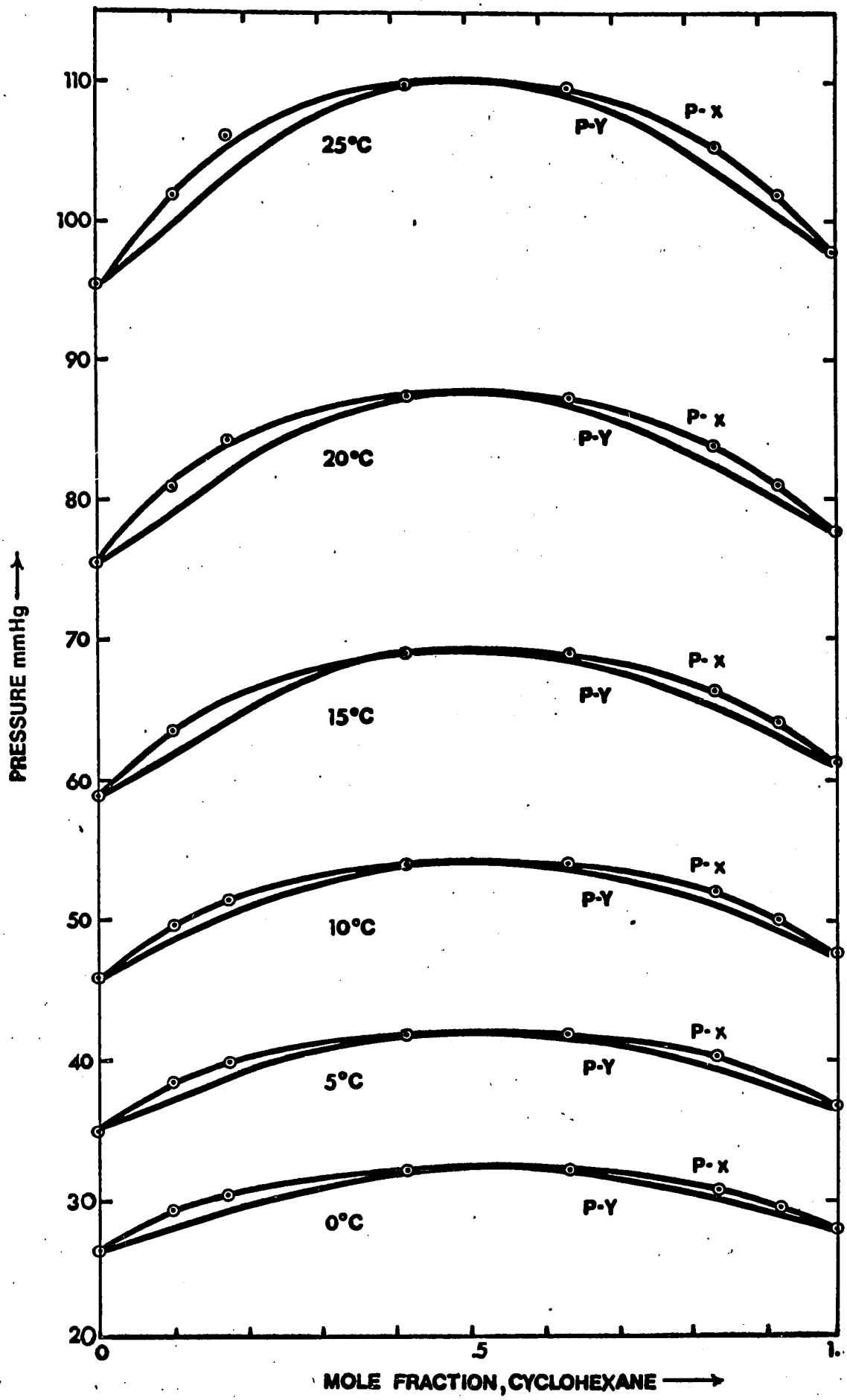

Fig. 2 - Total Vapor Pressure-Composition Diagram for the Cyclohexane-Benzene System

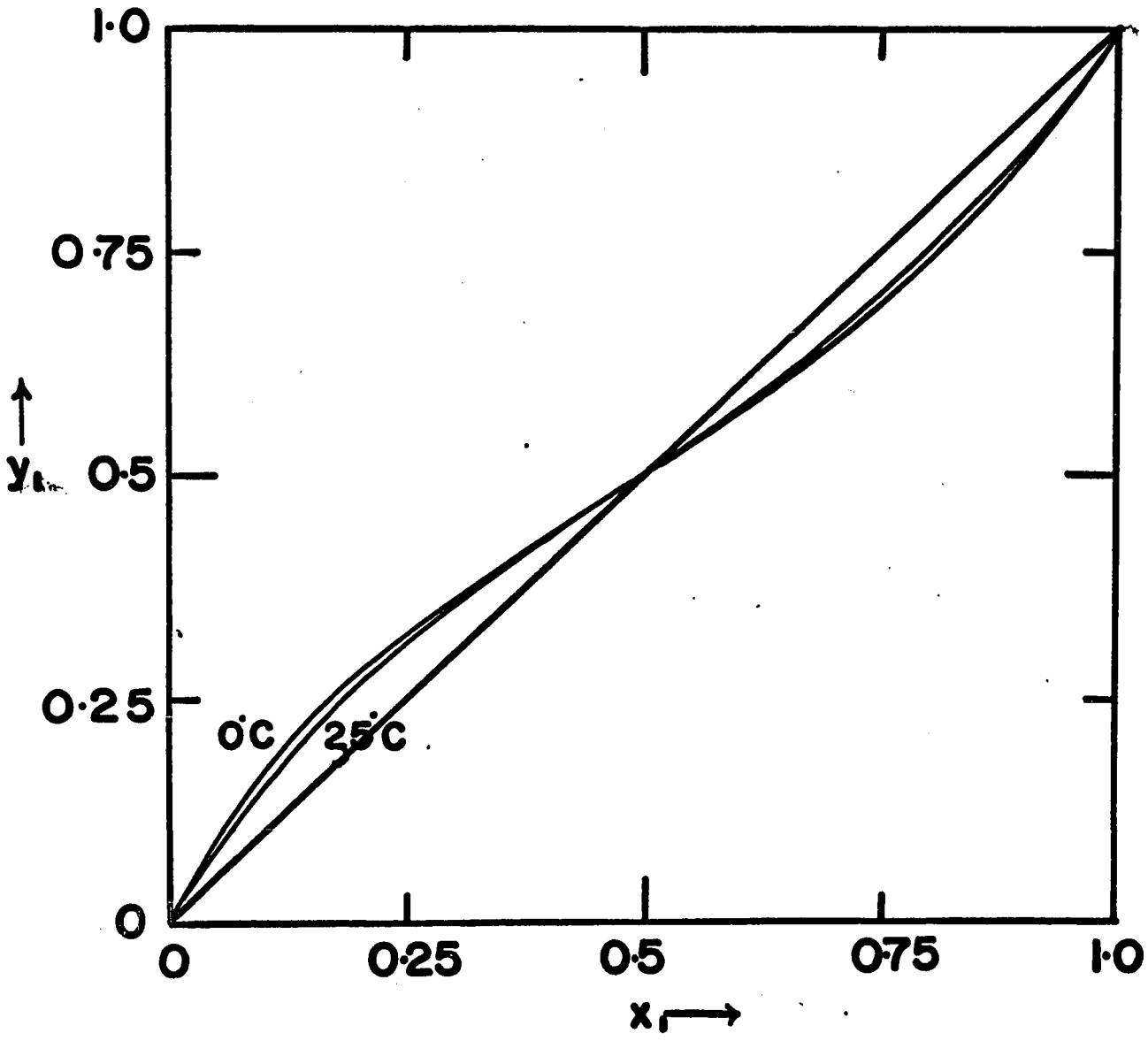

Fig. 3 - Vapor-Liquid Composition Diagram for the Cyclohexane-Benzene System

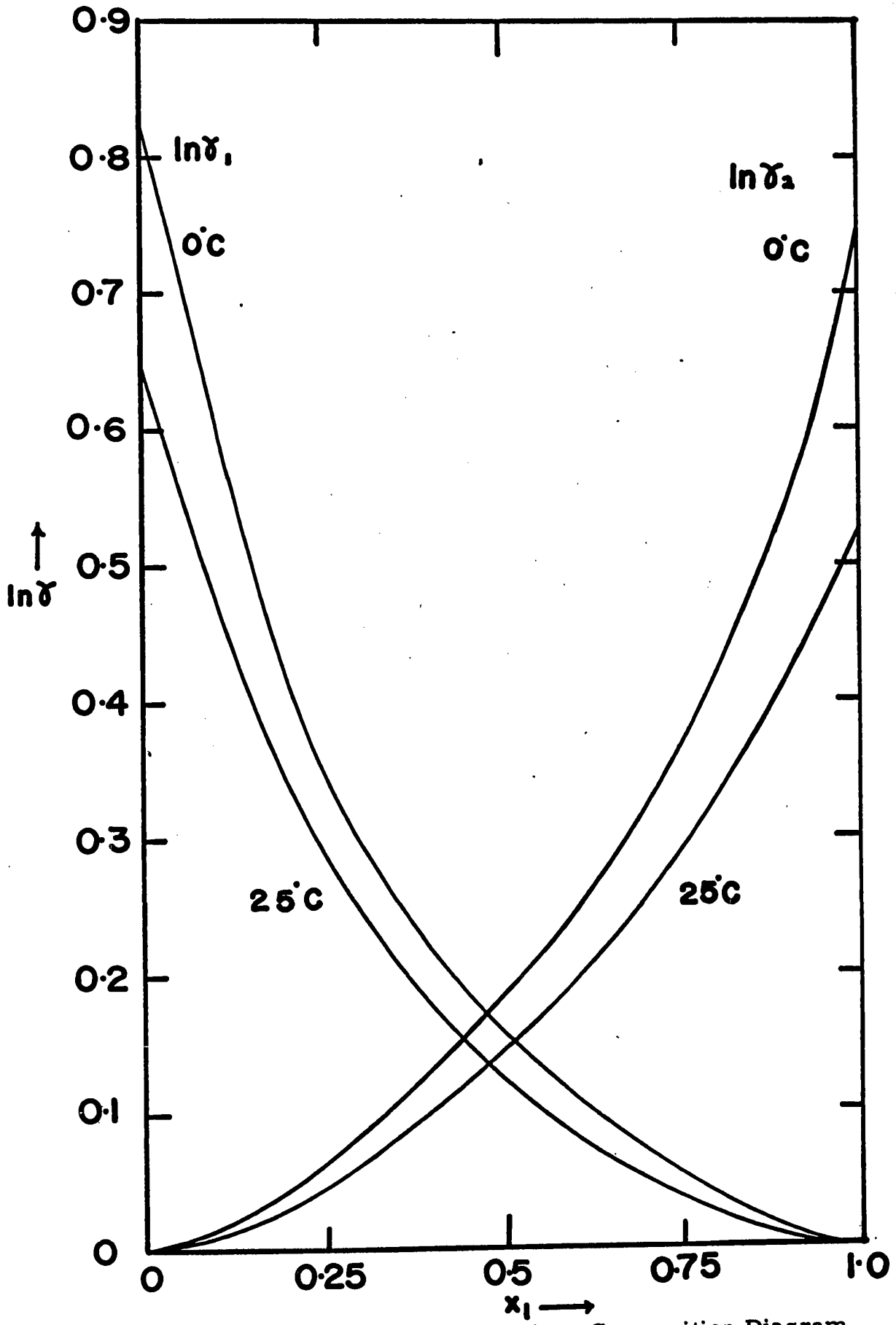

Fig. 4 - Liquid Activity Coefficient-Composition Diagram for the Cyclohexane-Benzene System

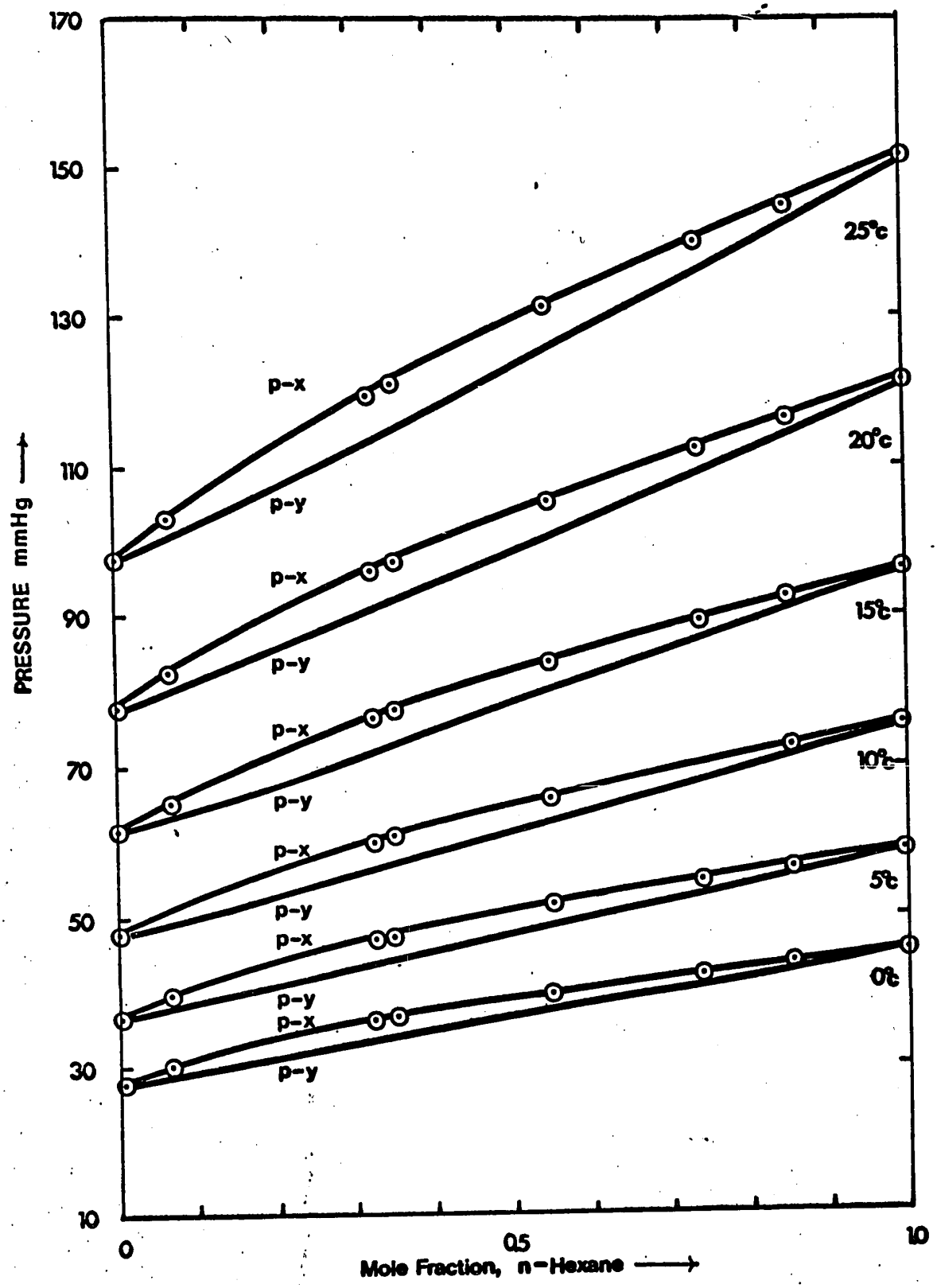

Fig. 5 - Total Vapor Pressure-Composition Diagram for the n-Hexane-Cyclohexane System

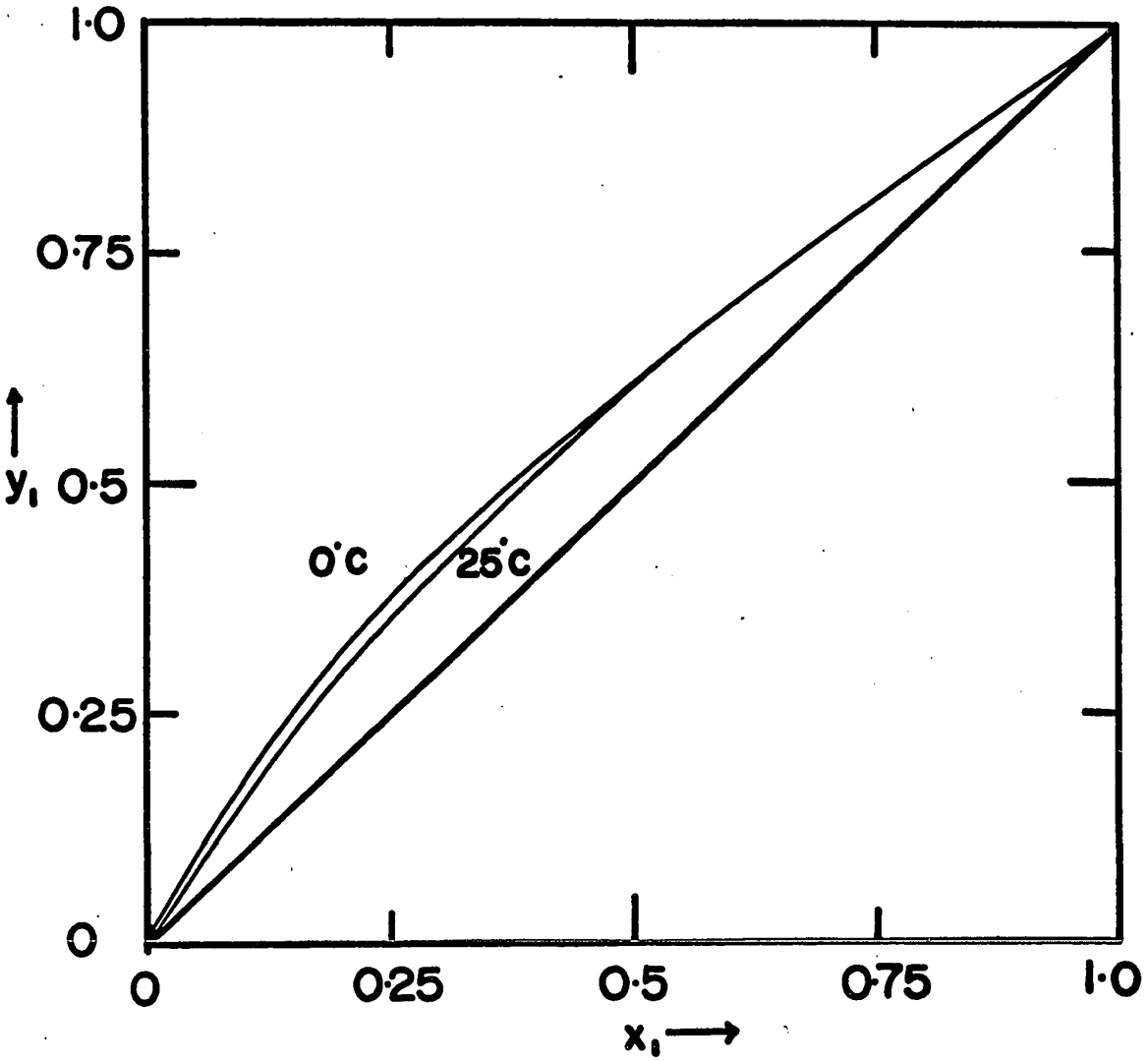

Fig. 6 - Vapor-Liquid Composition Diagram for the n-Hexane-Cyclohexane System

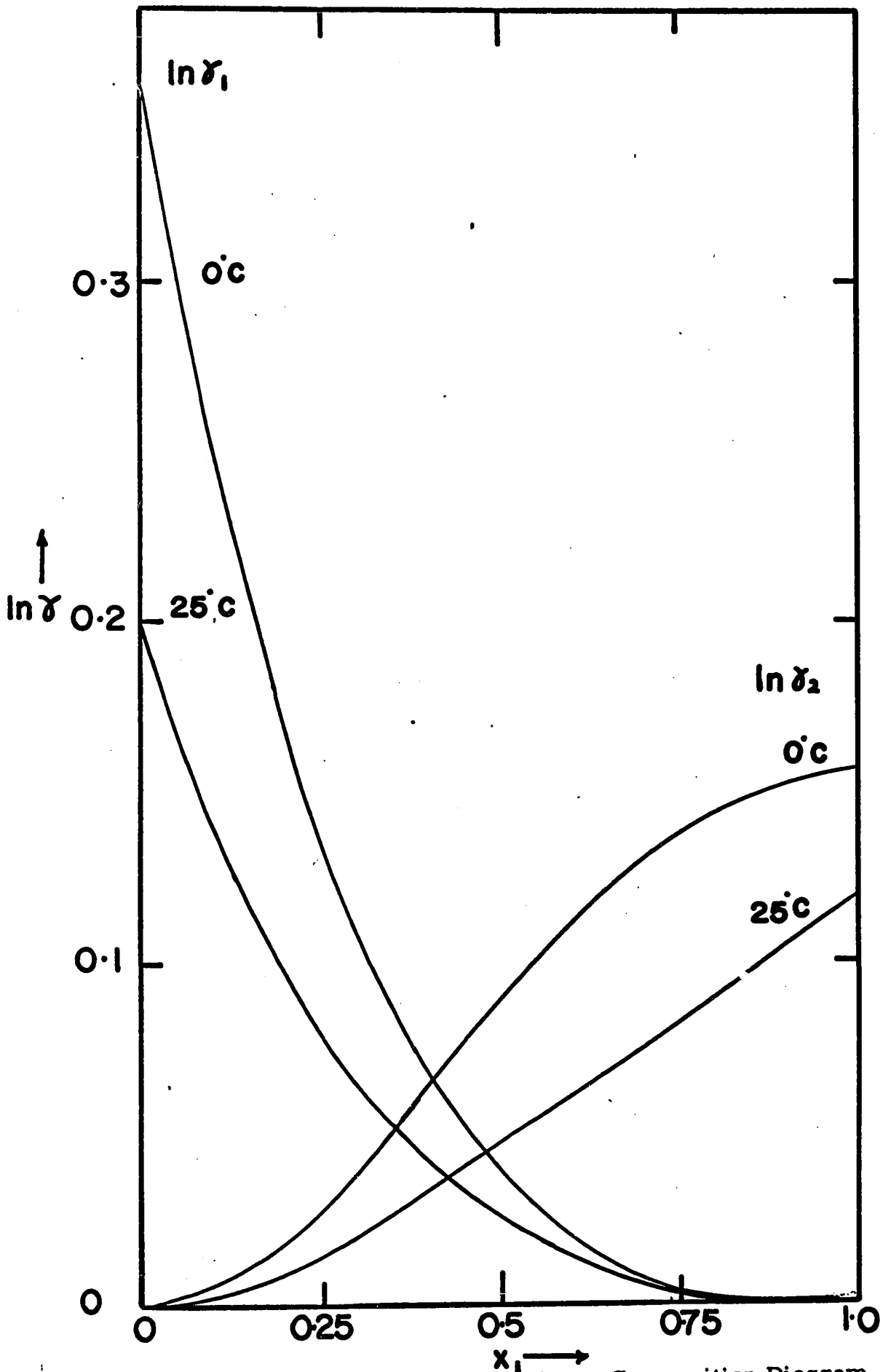

Fig. 7 - Liquid Activity Coefficients-Composition Diagram for n-Hexane-Cyclohexane System

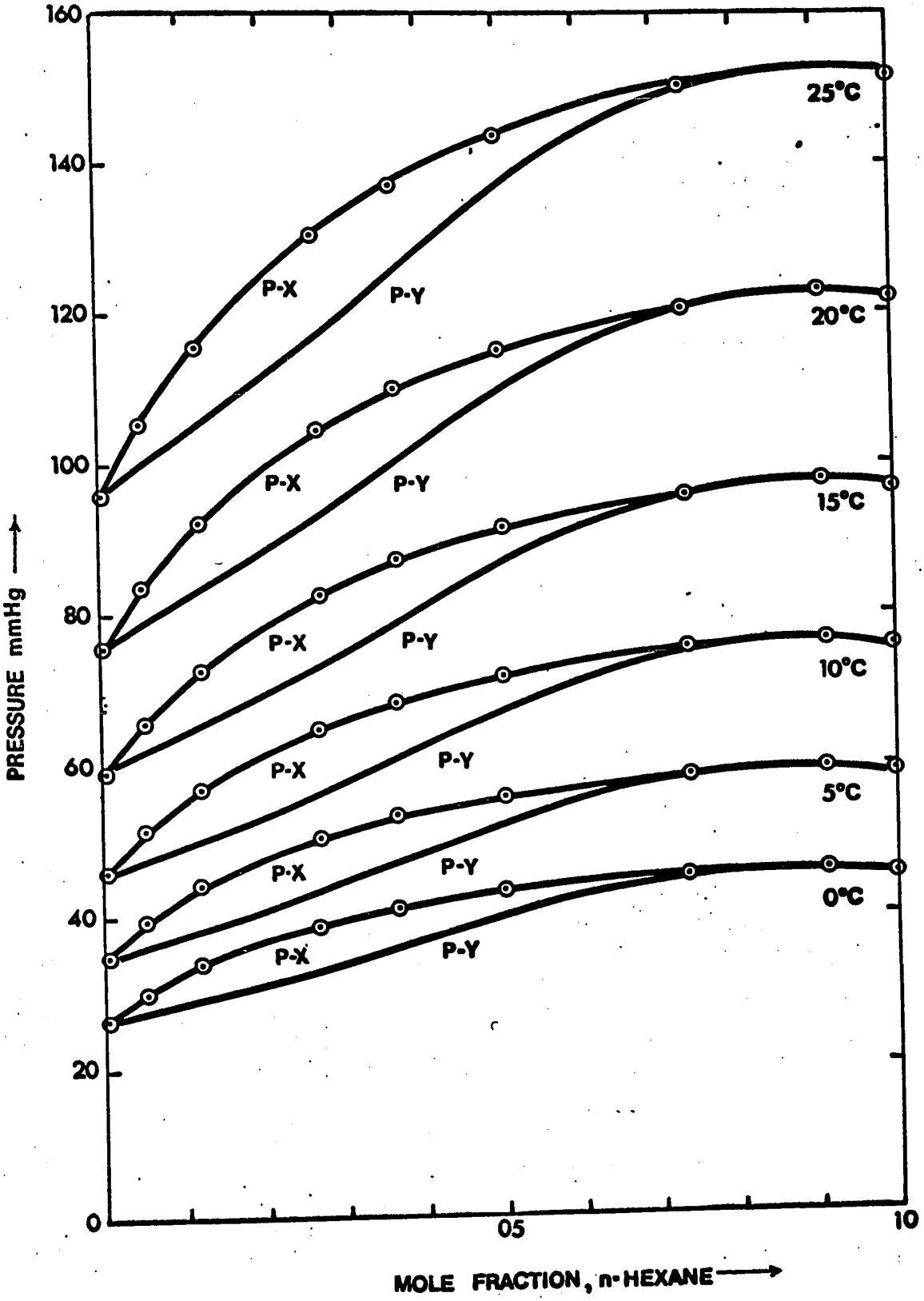

Fig. 8 - Total Vapor Pressure-Composition Diagram for the n-Hexane-Benzene System

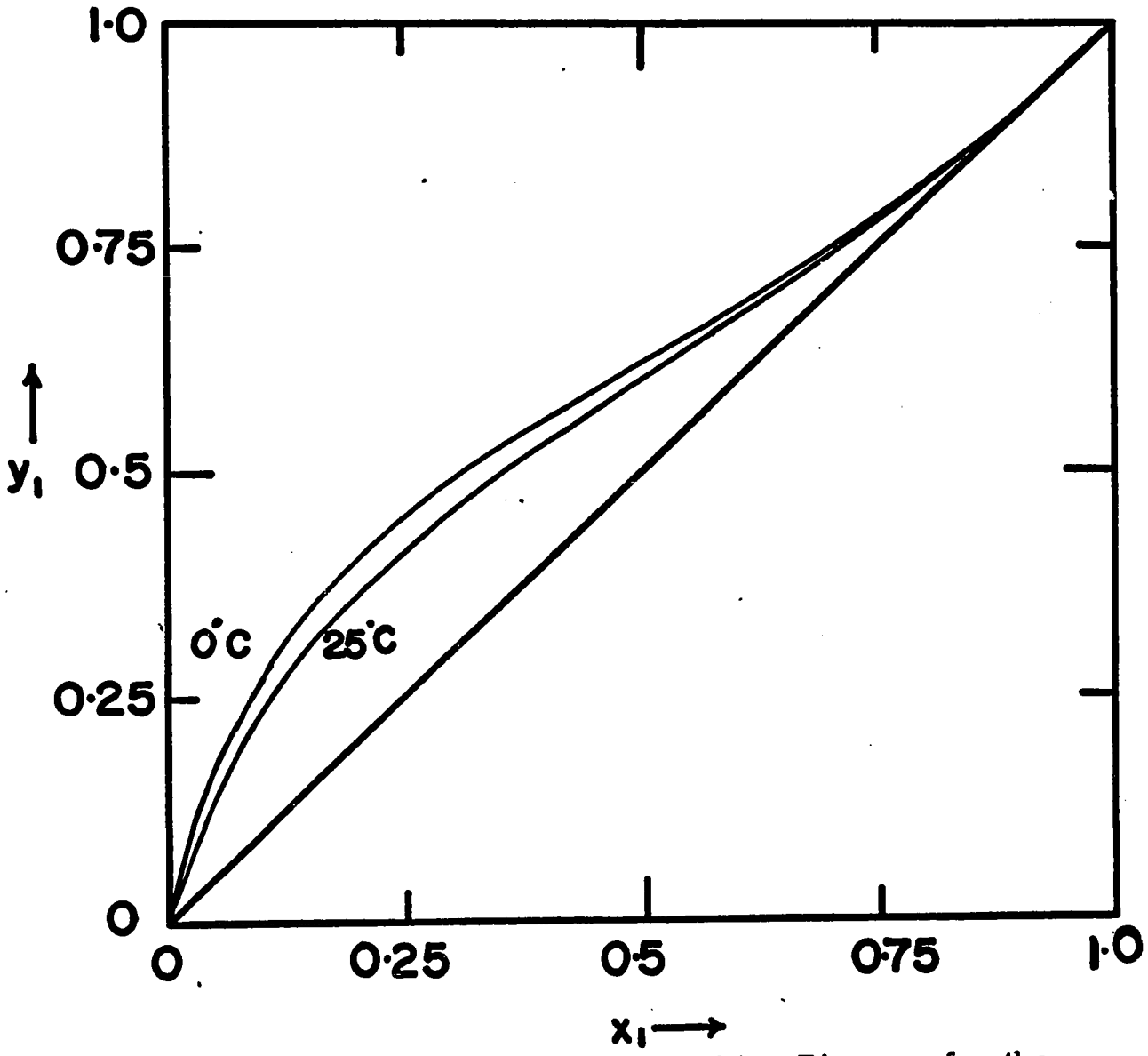

Fig. 9 - Liquid-Vapor Composition Diagram for the n-Hexane-Benzene System

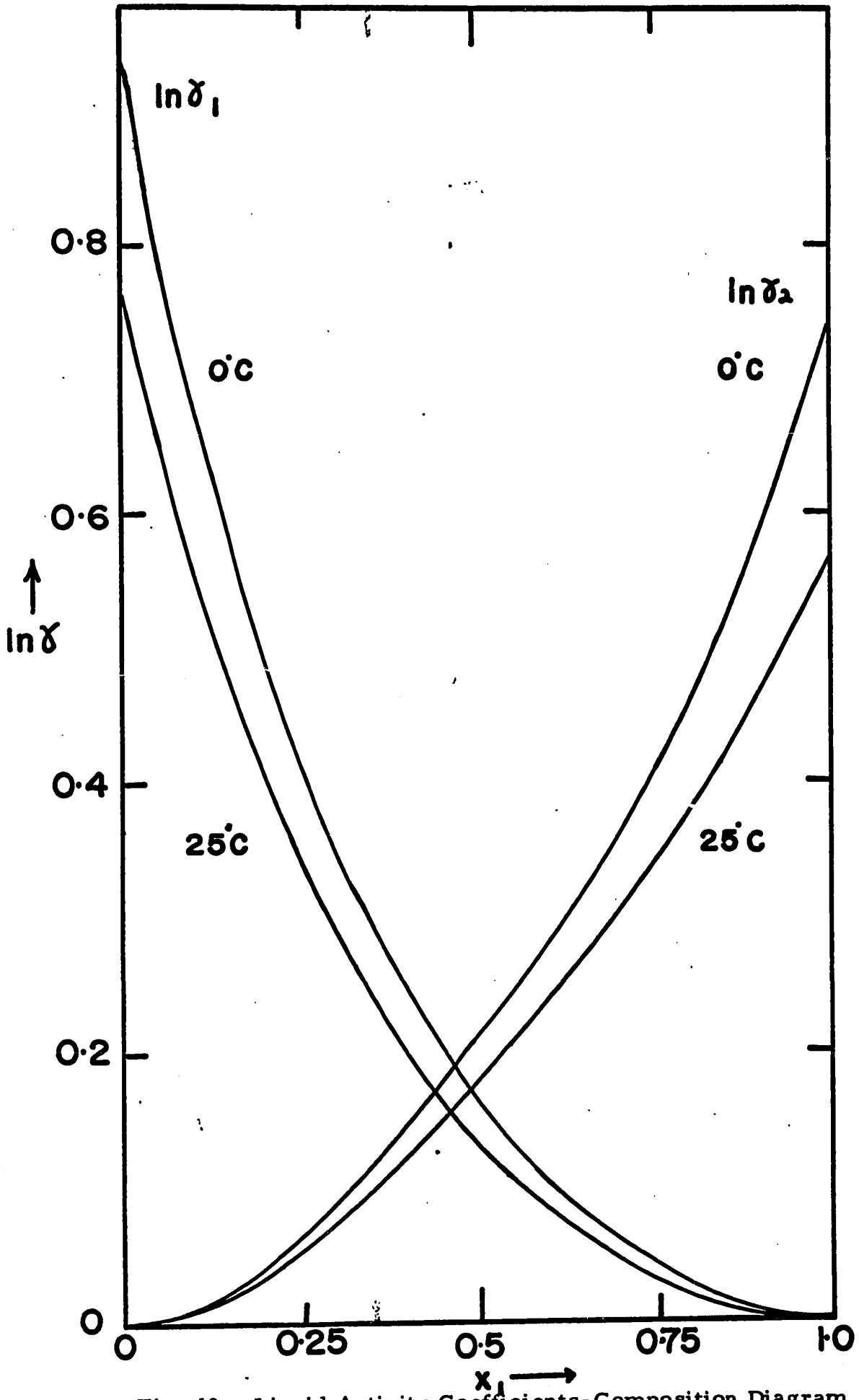

Fig. 10 - Liquid Activity Coefficients-Composition Diagram for the n-Hexane-Benzene System

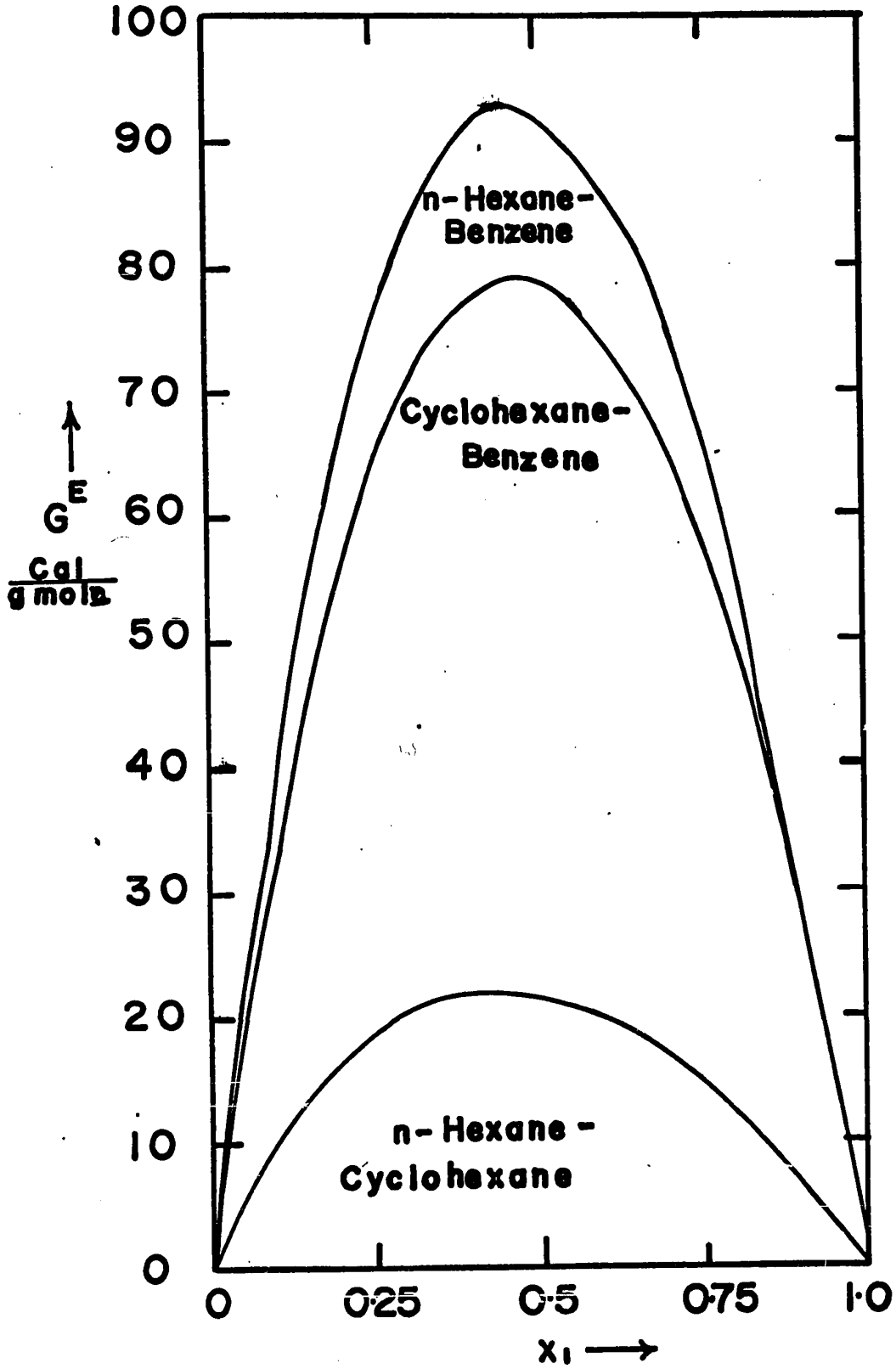

Fig. 11 - Excess Gibbs Free Energies at 25°C for the three binary systems

CHAPTER VI

DISCUSSION OF THE RESULTS

A. Vapor Pressures of Mixtures at Constant Composition

Total vapor pressures of pure components n-hexane, cyclohexane and benzene measured were compared with the vapor pressures calculated from the Antoine constants reported in the literature [1, 30]. The agreement is extremely good, and the deviation is less than 0.03 mm Hg. In the binary system of cyclohexane-benzene, it was observed that the freezing points of the mixtures are lower than those of the pure components. The vapor pressures measured were correlated by the Antoine equation and the standard deviation of the fitting is very small, less than 0.15 mm Hg.

B. Vapor-Liquid Equilibria at Constant Temperature

Total vapor pressures at constant compositions were interpolated using the calculated Antoine equation constants at 0°, 5°, 10°, 15°, 20° and 25°C for the three binary systems. The vapor compositions, liquid-phase activity coefficients, calculated total vapor pressures and Gibbs excess free energies were calculated from the interpolated data, based on the results of the indirect method. At the same temperatures 0°, 5°, 10° 15°, 20° and 25°C, the constants for correlating total vapor pressures as a function of liquid compositions were calculated and the vapor compositions were calculated by the direct method. As observed from Tables 8, 9, and 10, the y and P values calculated, agree very well with each other, with the standard deviations are less than 0.006 mole fraction and 0.3 mm Hg respectively.

C. Comparison with Literature Data

1. Comparison between the Interpolated and Literature Data at Isothermal Conditions

The total vapor pressures of the cyclohexane-benzene system at 10°C were compared with the results from the reference [6] as shown in Figure 12. Both data agree extremely well as observed from Figure 12.

The vapor pressures of the n-hexane-benzene at 25°C was compared with recent report of Smith and Robinson [9] as shown in Figure 13. It is observed that the comparison are quite satisfactory, except in the high concentration region of n-hexane. This is perhaps due to the fact that the vapor pressure of the pure n-hexane employed is higher than the value obtained from this investigation and the literature values [1, 30]. When the vapor pressures of this work and of the work of Smith and Robinson [9] were individually fitted by means of Eq. (32), the maximum value of P and x_1 obtained agrees closely (154.13 mm Hg, 0.904 mole fraction and 152.62 mm Hg, 0.901 mole fraction respectively).

2. Comparison Between the Extrapolated and Literature Data

In combining with some of the literature data, a new set of Antoine equation constants at extended temperature range from 0°to 80°C were calculated and are given in Table 11. The percent deviation of the fitting is less than 0.55 %. From the Antoine equation constants the total vapor pressures at isothermal conditions and the bubble-point temperatures at isobaric conditions were calculated and compared with the literature data, as shown in Table 12. The graphical presentations are shown in Figure 14-19. They all agree extremely well, as observed in all the figures. Maybe, due to the

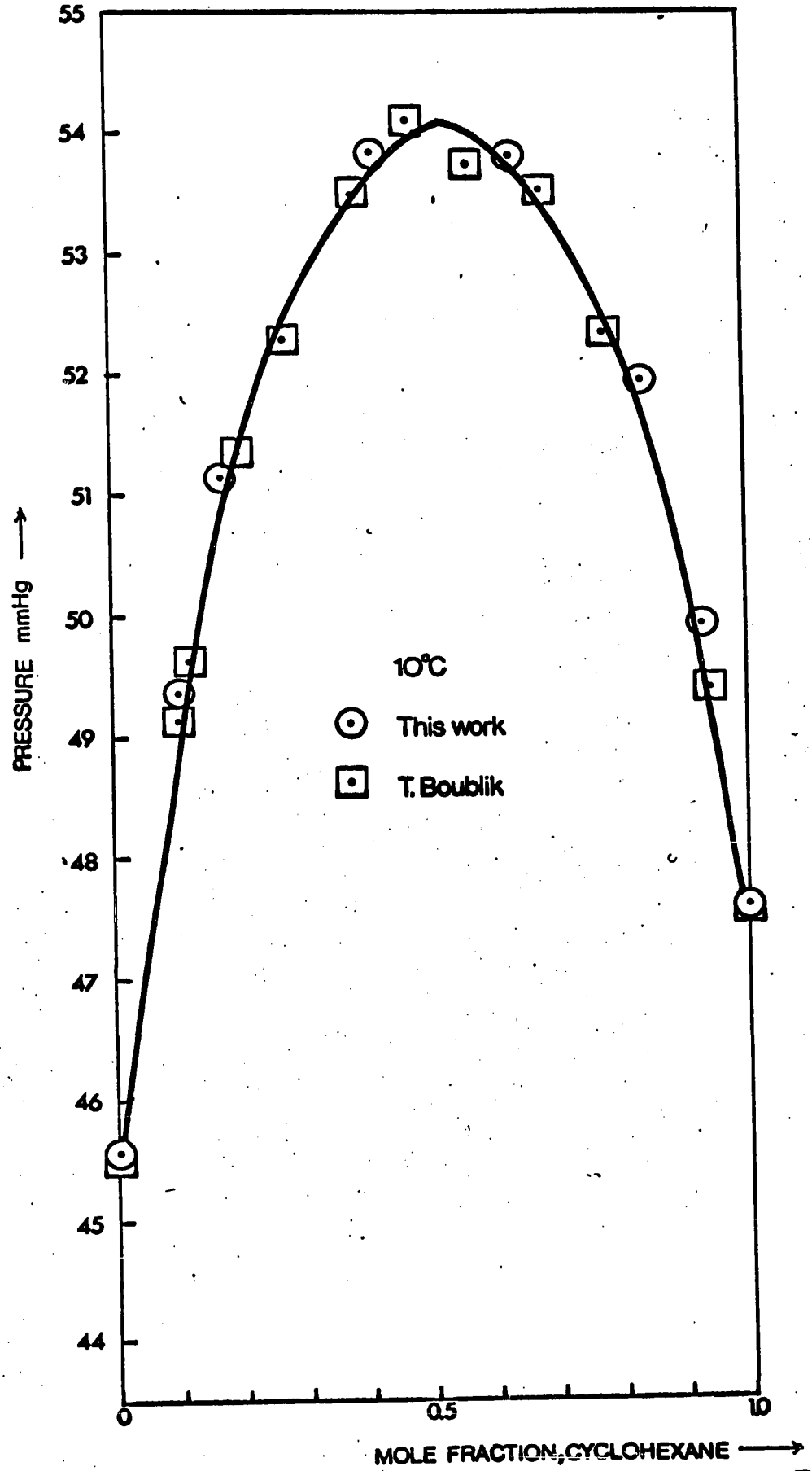

Fig. 12 - Comparison of the Interpolated Total Vapor Pressure Values with Literature Data for the System Cyclohexane-Benzene at 10°C (6)

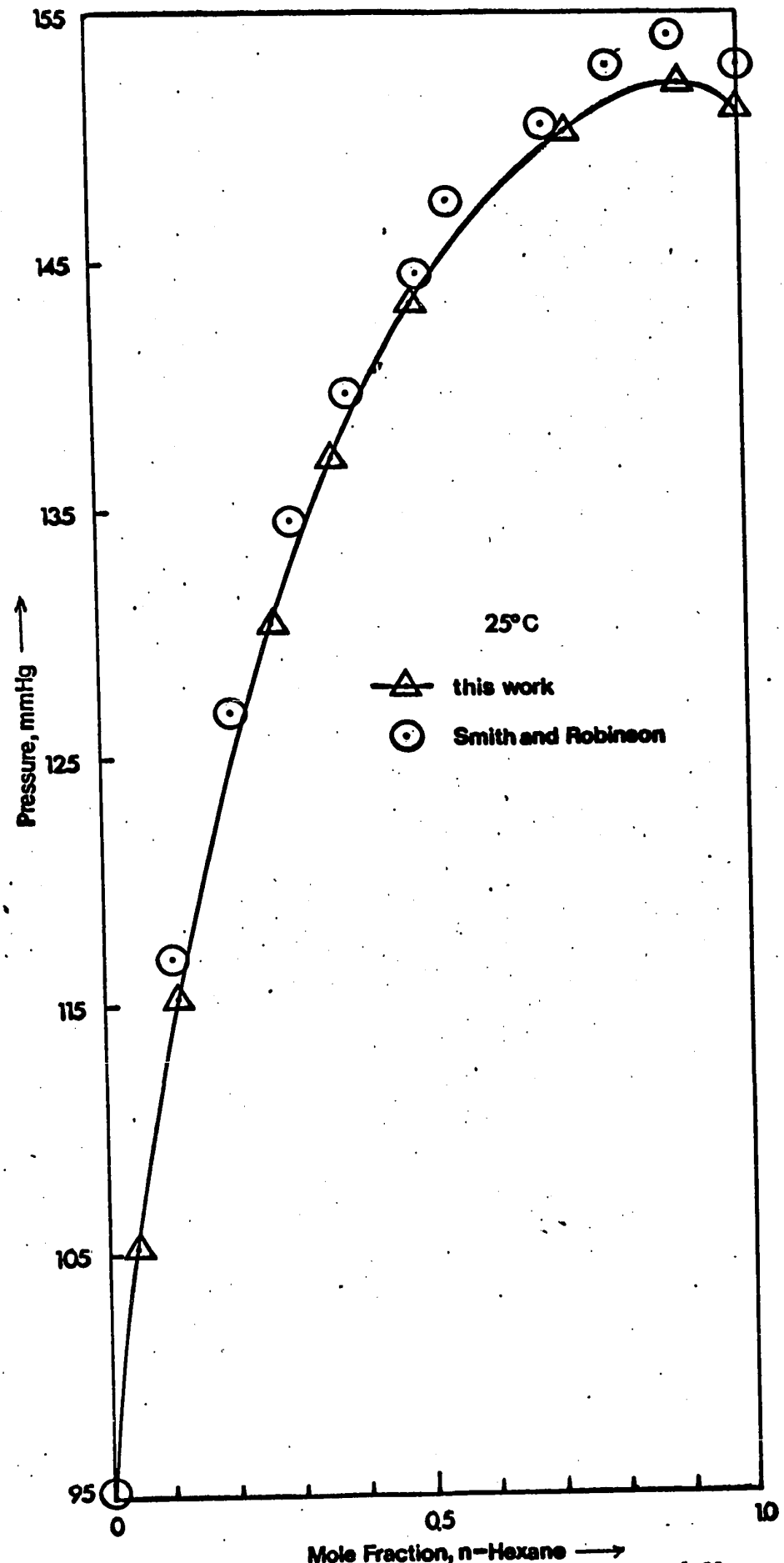

Fig. 13 - Comparison of the Interpolated Total Vapor Pressure Values with Literature Data for the System n-Hexane-Benzene at 25°C(7)

presence of impurities, the P value of n-hexane of Susarev [5] is slightly higher than that of this work and the value reported from Scatchard [1] and Dreisbach [30].

3. Azeotropes

Azeotropes were observed to be present in the benzene containing systems: cyclohexane-benzene and n-hexane-benzene. The correlated constants and the numerical values of the azeotropic concentration and total vapor pressure calculated by differentiation of of Eq. (32) are tabulated in Table 13 and 7. As observed from Table 13, the comparison of the azeotropic composition and azeotropic total vapor pressure between this work and the calculated literature values agree very well, with the difference less than 0.02 mole fraction and 1.5 mm Hg respectively.

TABLE 11

Correlation of Total Vapor Pressure Data at Constant Liquid Compositions by Means of the Antoine Equation over the Temperature Range from 0° to 80°C

x_1	a	b	c	Dev mmHg	Dev %	References
Cyclohexane-Benzene						
0.000	6.927628	1222.099	221.942	1.25	0.19	1, 2, 3, 4
0.102	6.999122	1268.769	229.141	0.70	0.18	
0.174	7.017695	1285.989	232.485	0.93	0.27	
0.418	6.963348	1253.913	229.661	0.91	0.20	
0.635	6.957421	1253.981	229.924	0.47	0.13	
0.838	6.977865	1275.377	232.346	0.63	0.16	
0.923	6.866721	1215.856	225.240	0.85	0.16	
1.000	6.706008	1129.255	214.501	0.55	0.27	
n-Hexane-Cyclohexane						
0.000	6.706008	1129.255	214.501	0.55	0.27	2, 5
0.064	6.584733	1071.424	209.518	0.83	0.84	
0.321	7.037570	1310.907	239.247	0.27	0.18	
0.349	6.866009	1211.571	228.236	0.33	0.14	
0.544	6.678382	1100.163	216.327	1.06	0.38	
0.736	6.752910	1125.475	219.304	0.84	0.24	
0.850	6.799194	1143.880	221.613	0.10	0.12	
1000	6.850457	1157.834	222.913	0.26	0.09	
n-Hexane-Benzene						
0.000	6.927628	1222.099	221.942	1.25	0.19	2, 7, 8, 10
0.048	6.981803	1260.889	229.147	1.52	0.35	
0.118	6.717801	1124.258	216.498	1.58	0.55	
0.269	6.704669	1109.485	216.778	1.10	0.34	
0.366	6.803830	1155.973	222.684	0.62	0.15	
0.501	6.880692	1189.042	226.664	0.59	0.15	
0.735	6.879121	1180.799	226.065	0.96	0.23	
0.910	6.887916	1184.030	226.630	0.72	0.16	
1.000	6.850457	1157.834	222.913	0.26	0.09	

TABLE 12

Comparison of Calculated Total Vapor Pressures from the Antoine Equation Constants of Table 11 with Literature Values

Cyclohexane-Benzene

	Isobaric		Isothermal	
x_1	760 mmHg t° C	759 mmHg	39.99°C P mmHg	69.98°C P mmHg
0.000	80.05	80.00	182.88	551.20
0.102	78.94	78.80	192.65	572.66
0.174	78.37	78.33	197.60	583.68
0.418	77.48	77.44	205.67	601.21
0.635	77.68	77.64	204.58	596.48
0.838	78.95	78.90	197.00	576.00
0.923	79.80	79.75	191.43	562.08
1.000	80.71	80.67	184.79	546.20

n-Hexane-Cyclohexane

x_1	760 mmHg	70°C
0.000	80.71	545.46
0.064	79.75	564.44
0.321	76.12	628.31
0.349	75.78	636.14
0.544	73.37	685.58
0.736	71.36	728.82
0.850	70.31	752.67
1.000	68.76	790.02

n-Hexane-Benzene

x_1	760 mmHg	30°C	40°C	50°C	60°C
0.000	80.05	119.38	182.85	271.44	391.80
0.048	78.31	130.69	198.17	291.65	417.90
0.118	76.51	143.51	216.12	315.62	448.47
0.269	73.37	161.73	242.03	351.42	496.70
0.366	71.98	169.46	253.05	366.94	518.27
0.501	70.61	177.01	264.08	382.74	540.54
0.735	69.26	185.26	276.13	399.82	564.14
0.910	68.85	188.00	280.02	405.25	571.55
1.000	68.76	187.27	279.64	405.47	572.69

TABLE 13

Constants for Correlation total vapor pressures as a function of Liquid Composition over a Temperature Range from 0° to 70°C

t°C	C_1	C_2	C_3	C_4	St Dev mmHg	Dev %	Max x_1	Max P mm Hg	Ref
Cyclohexane-Benzene									
39.99	88.8817	- 6.37889	16.6930		0.08	0.04	.491	206.06	1
					0.30	0.15	.488	206.10	*
69.98	211.040	-14.6222	27.0566		0.32	0.05	.462	600.63	1
					0.63	0.11	.462	601.07	*
n-Hexane-Cyclohexane									
70	14.0013	23.5485	-70.7333	-178.197	2.74	0.39			5
					1.97	0.28			*
n-Hexane-Benzene									
30	92.3274	-47.3497	29.1300		0.51	0.35	.968	187.70	8
					0.51	0.33	.942	187.99	*
40	130.229	-63.5619	47.3866		0.53	0.22	.945	279.96	8
					0.41	0.17	.435	280.18	*
50	177.831	-70.7001	58.3663	- 27.518	0.74	0.21	.935	406.26	8
					0.47	0.13	.941	406.07	*
60	235.164	-71.6639	70.3216	- 48.434	0.88	0.18	.926	574.53	8
					0.73	0.14	.946	573.50	*
25	82.7678	-37.0834	47.9422	- 20.389	0.74	0.55	.904	154.13	9
					0.46	0.38	.901	152.62	*

* This Work

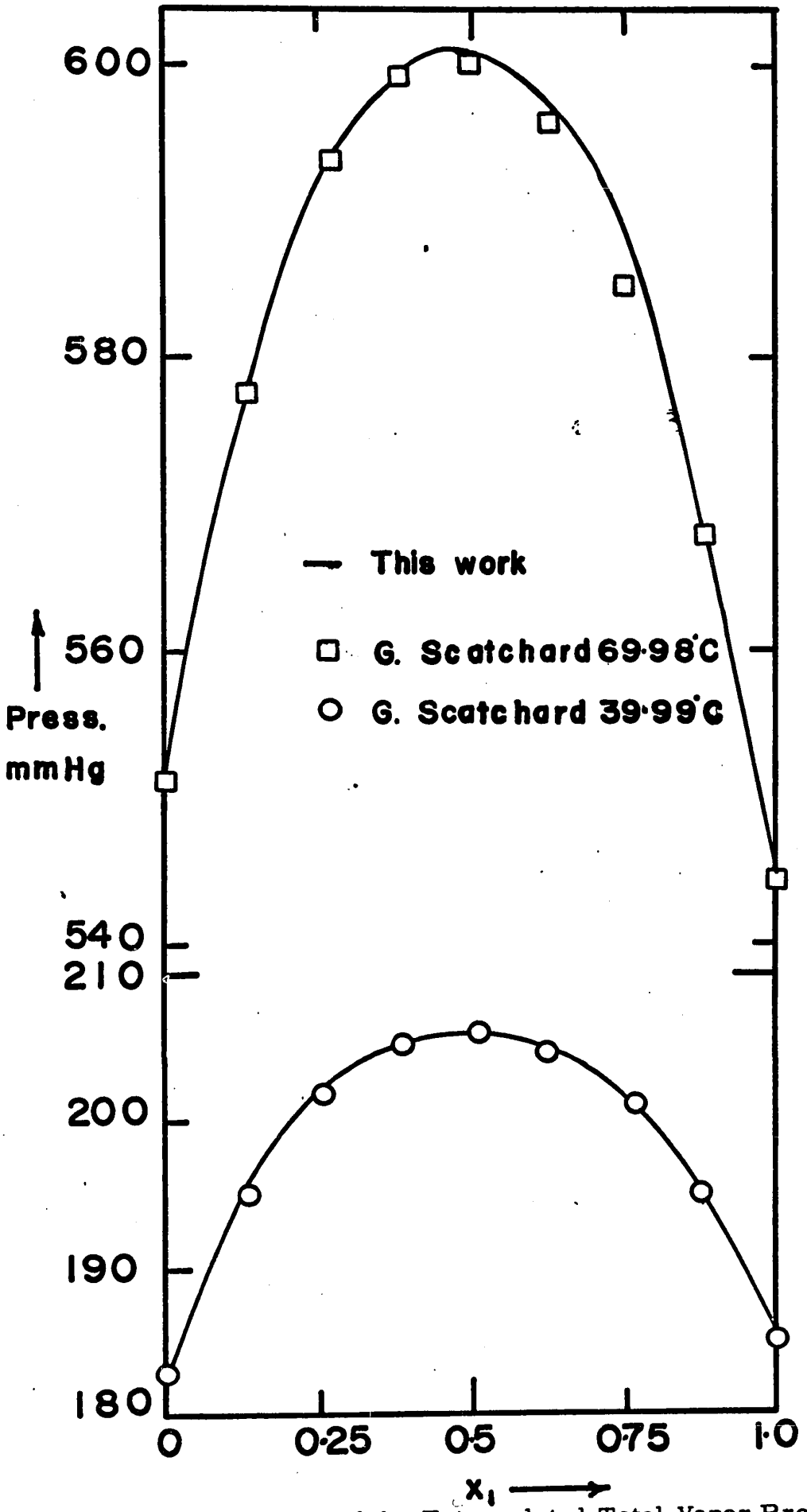

Fig. 14 - Comparison of the Extrapolated Total Vapor Pressure Values with Literature Data for the System Cyclohexane-Benzene at 39.99° and 69.98°C (1)

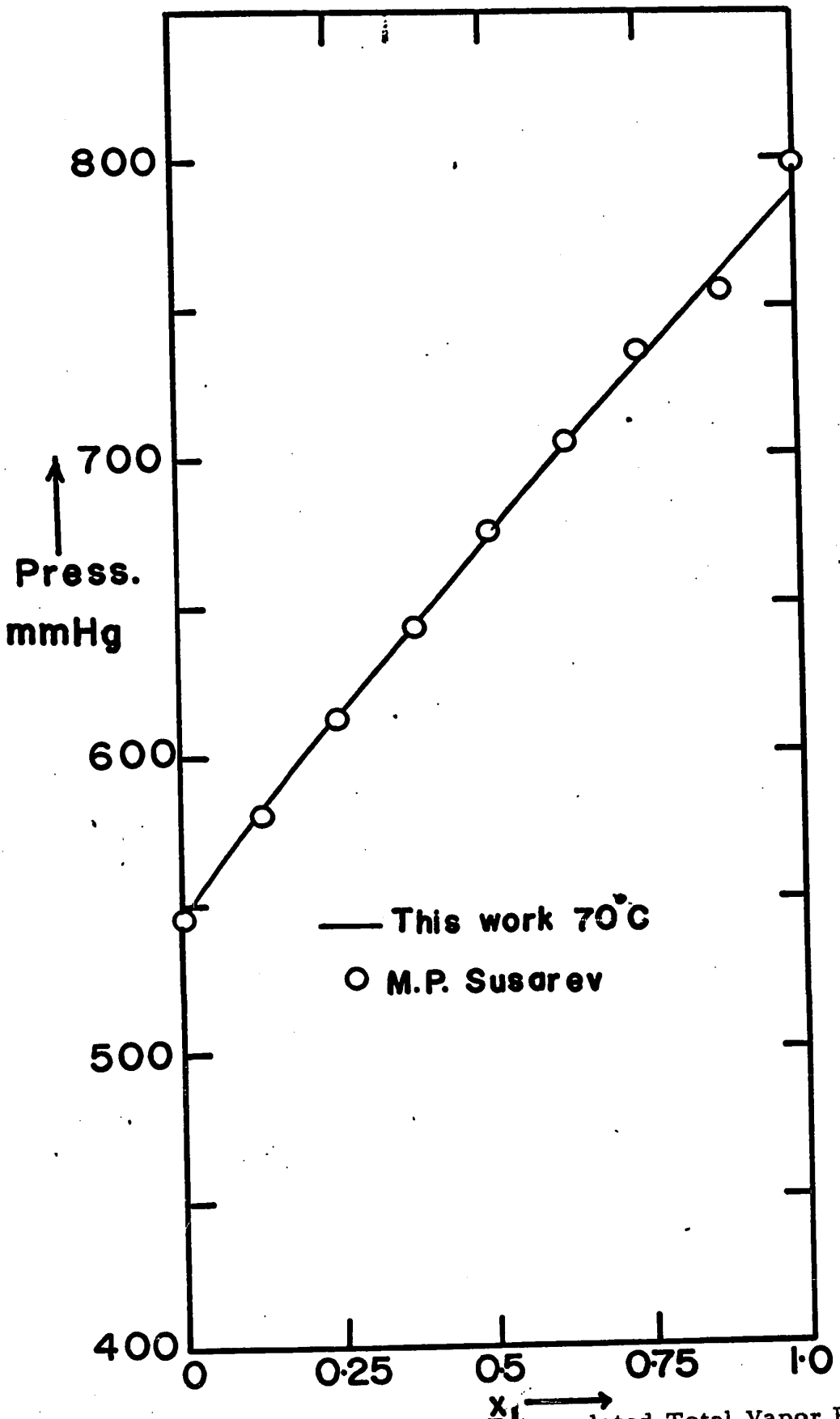

Fig. 15 - Comparison of the Extrapolated Total Vapor Pressure Values with Literature Data for the System n-Hexane-Cyclohexane at 70°C (5)

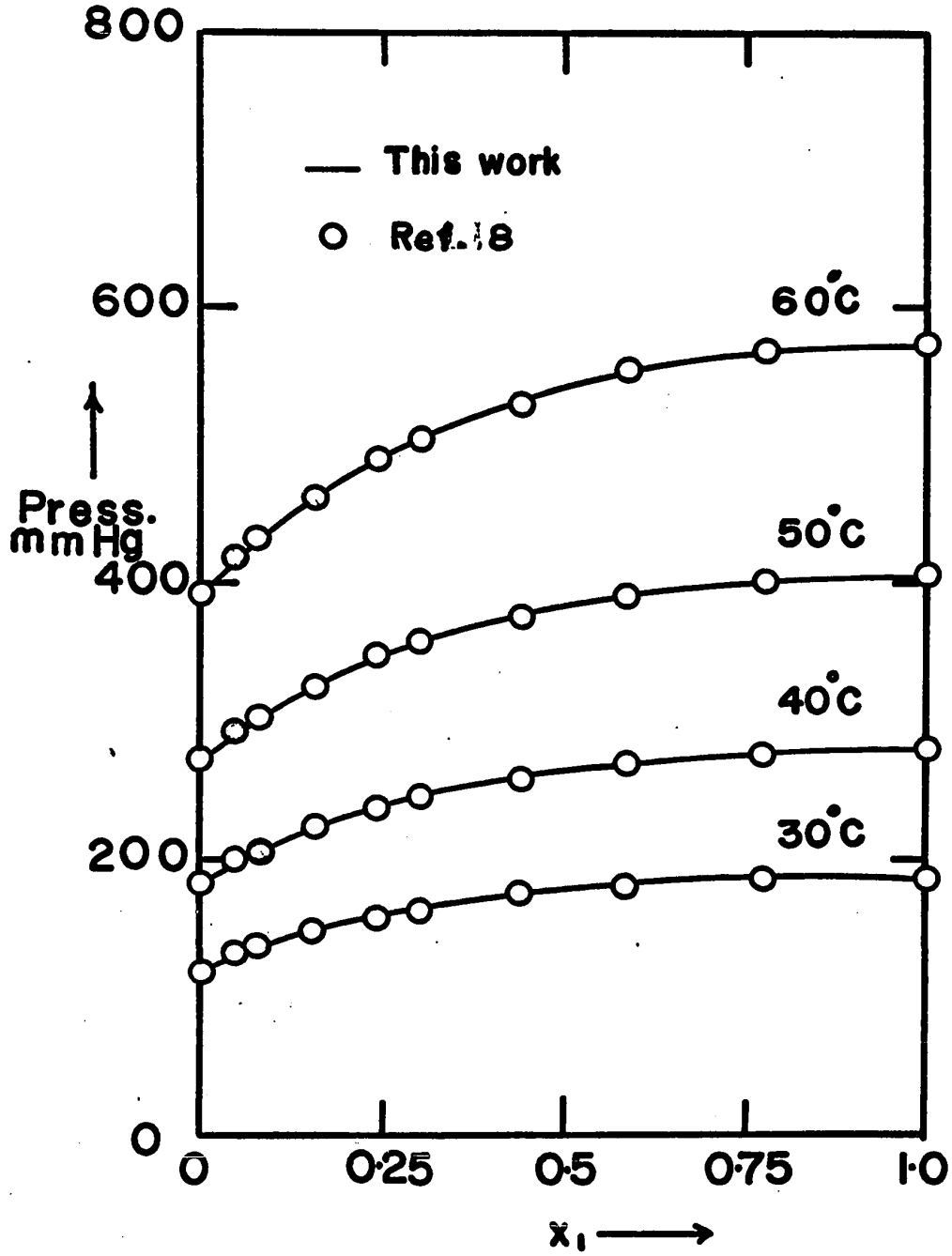

Fig. 16 - Comparison of the Extrapolated Total Vapor Pressures Values with Literature Data for the System n-Hexane-Benzene at 30°, 40°, 50° and 60°C

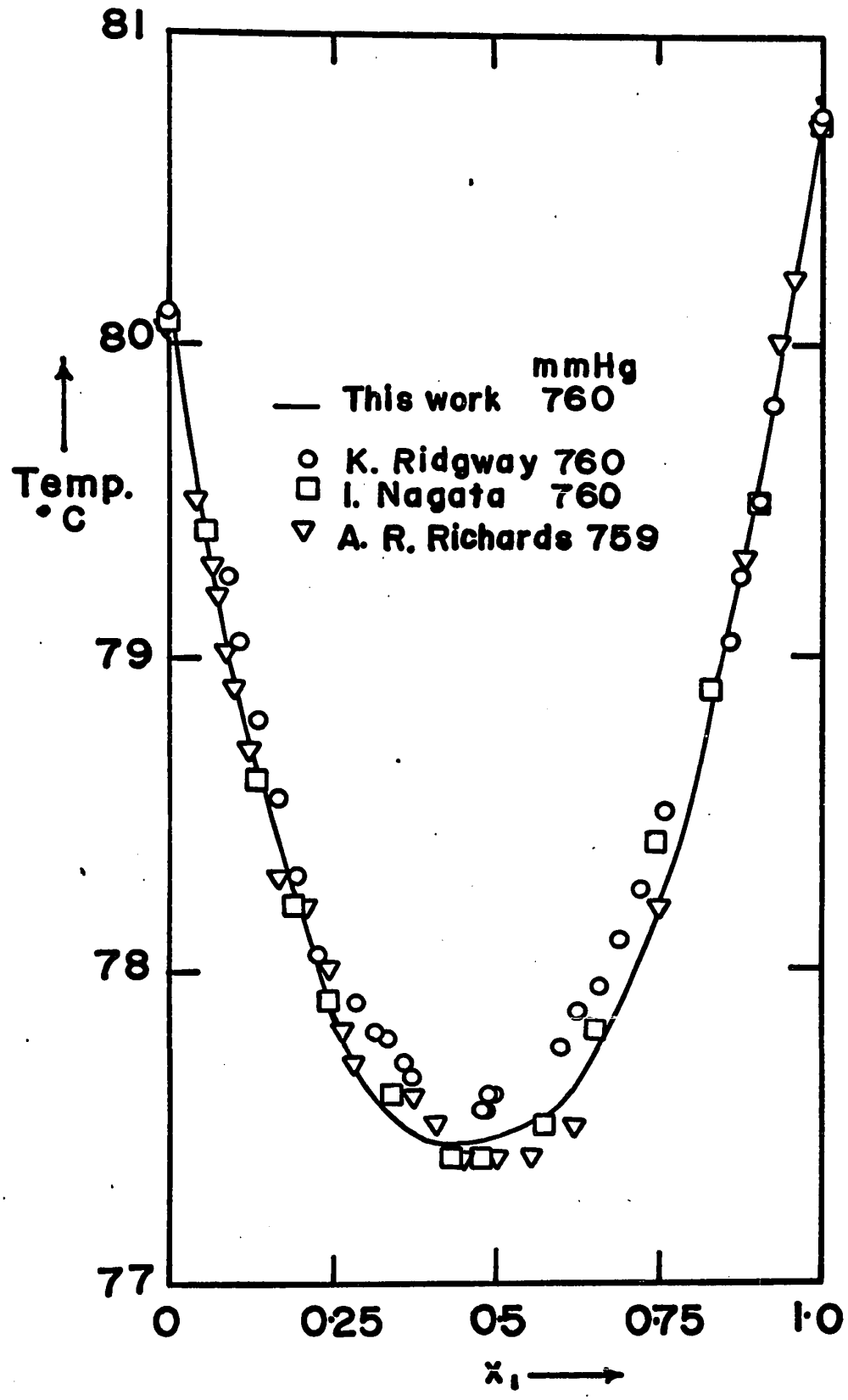

Fig. 17 - Comparison of the Extrapolated Bubble - Point Temperature Values with Literature Data for the System Cyclohexane-Benzene at 759 and 760 mm Hg. (2, 3, 4)

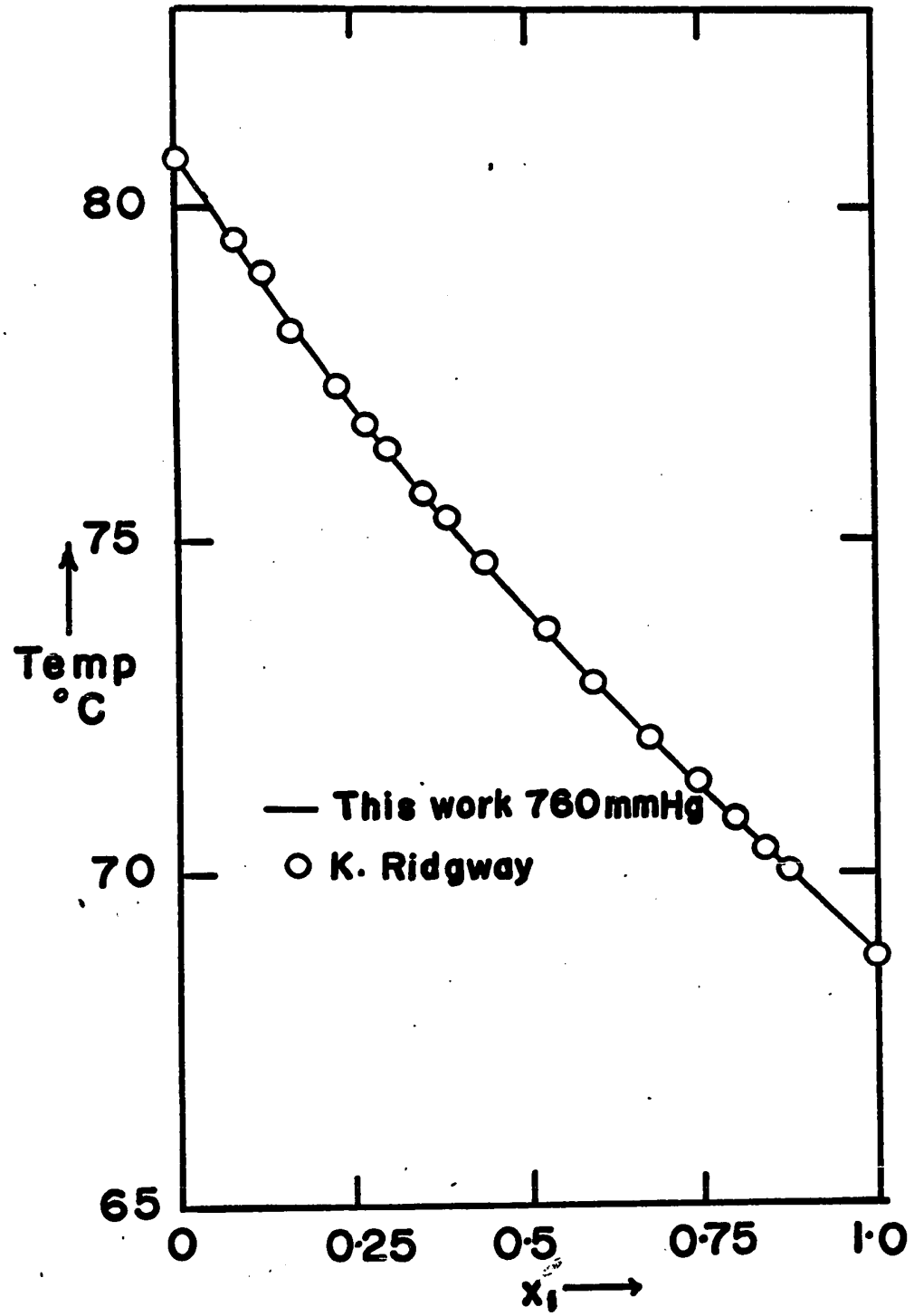

Fig. 18. - Comparison of the Extrapolated Bubble-Point Temperature Values with Literature Data for the System n-Hexane-Cyclohexane at 760 mm Hg [2]

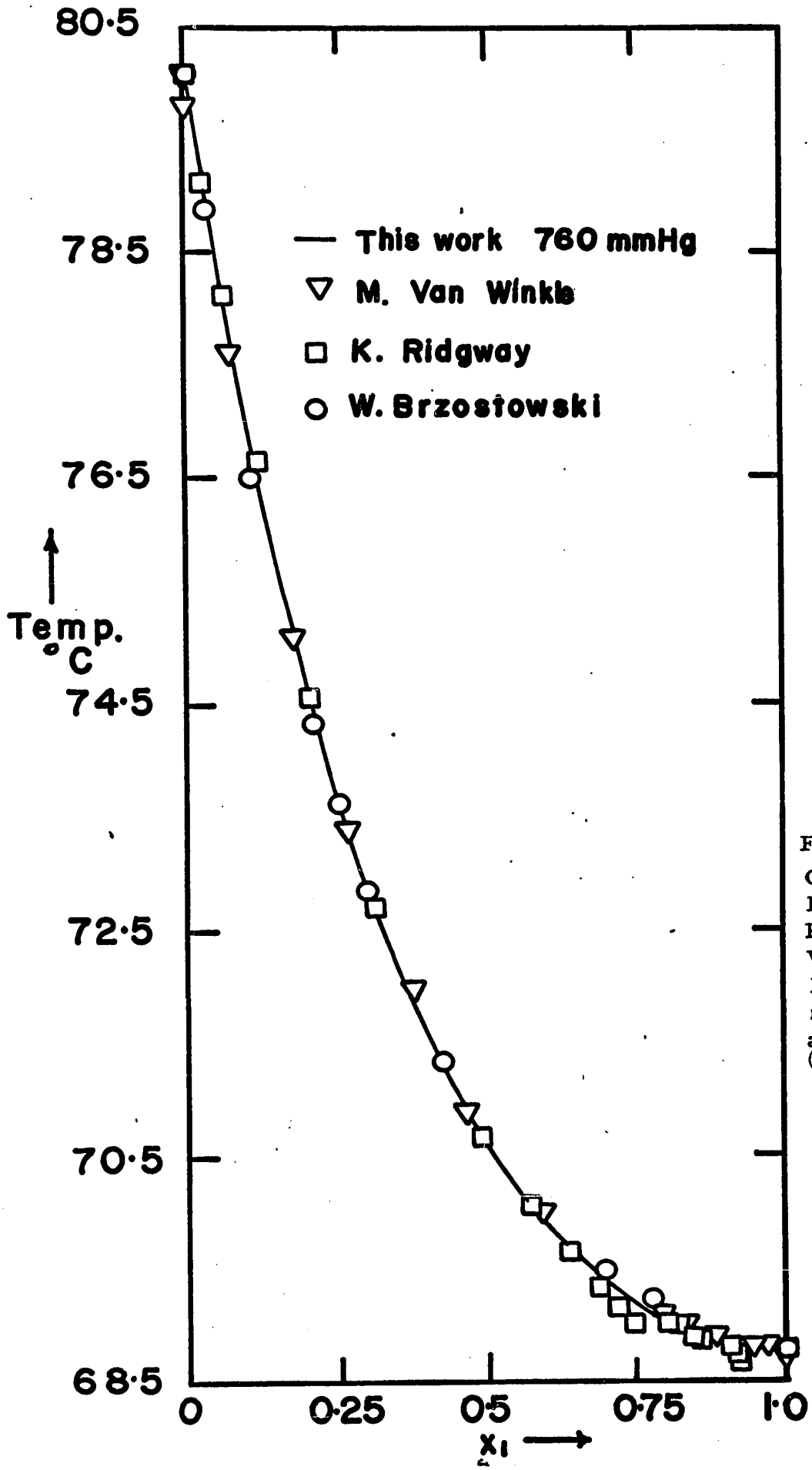

Fig. 19 - Comparison of the Extrapolated Bubble-Point Temperature Values with Literature Data for the System n-Hexane-Benzene at 760 mm Hg (10, 2, 7)

CHAPTER VII

CONCLUSION

The design and operation of the static apparatus is very satisfactory. Vapor-liquid equilibrium data for the cyclohexane-benzene, n-hexane-cyclohexane and n-hexane-benzene systems were obtained at 0°, 5°, 10°, 15°, 20° and 25°C. The values so determined were smoothed and correlated by both direct and indirect methods. The smoothed and correlated results of those three systems are in good agreement with all the available literature data. The azeotropic points were observed in the two benzene containing systems.

CHAPTER VIII

NOMENCLATURE

a, b, c,	=	Antoine constants
C_1, C_2, C_3	=	constants, Equation 32
B, C, D,	=	Redlich-Kister parameters
f	=	fugacity
G^E	=	molal excess Gibbs free energy
P	=	total vapor pressure
p	=	vapor pressure of pure component
R	=	gas constant
T	=	temperature in °K
t	=	temperature in °C
V	=	liquid molal volume of pure component
x	=	mole fraction in liquid phase
y	=	mole fraction in vapor phase
z	=	compressibility factor
β_{11}, β_{22}	=	second virial coefficient of pure component 1 and 2, respectively
β_{12}	=	cross second virial coefficient
γ	=	activity coefficient
δ	=	defined in equation 15
φ	=	fugacity coefficient

Subscripts

1, 2, i, j = components

CHAPTER IX

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CHAPTER X

APPENDIX

		PAGE
I	CALIBRATION OF THE THERMOPILE.....	62
II	CALIBRATION OF THE PRESSURE GAUGE	66
III	DENSITY-LIQUID COMPOSITION DATA FOR THE THREE BINARY SYSTEMS	74
IV	COMPUTER PROGRAM FOR THE EVALUATION OF THE ANTOINE EQUATION CONSTANTS	87
V	COMPUTER PROGRAM FOR THE EVALUATION OF THE TOTAL VAPOR PRESSURE CORRELATION CONSTANTS.....	95
VI	COMPUTER PROGRAM FOR THE EVALUATION OF THE REDLICH-KISTER CONSTANTS AND THE CALCULATION OF y, γ AND Pcalc BY THE INDIRECT METHOD	111
VII	COMPUTER PROGRAM FOR THE EVALUATION OF THE VAPOR COMPOSITION BY THE DIRECT METHOD	118
VIII	PHYSICAL PROPERTIES	128

APPENDIX I

Calibration of the 5-junction Copper Constantin Thermopile

t°C	EMF (μv)
2.867	559
3.519	686
5.928	1157
8.758	1715
11.866	2331
14.348	2827
16.235	3204
20.000	3954
23.282	4621
24.541	4885
28.178	5630
30.250	6058

0.39540000E 04 0.20000000E 02
0.48850000E 04 0.24540985E 02
0.32040000E 04 0.16234985E 02
0.46310000E 04 0.23281998E 02
0.28270000E 04 0.14348000E 02
0.23310000E 04 0.11865999E 02
0.17150000E 04 0.87579994E 01
0.11570000E 04 0.59279995E 01
0.60580000E 04 0.30250000E 02
0.56300000E 04 0.28177994E 02
0.68600000E 03 0.35189991E 01
0.55900000E 03 0.28669996E 01
0.44041187E 03-0.14167888E 06 0.17402000E-02
1

	3954.0	3962.1	-8.1	-0.20	20.00
	4885.0	4884.9	0.1	0.00	24.54
	3204.0	3203.4	0.6	0.02	16.23
	4631.0	4628.2	2.8	0.06	23.28
	2827.0	2825.3	1.7	0.06	14.35
	2331.0	2330.4	0.6	0.03	11.87
	1715.0	1714.3	0.7	0.04	8.76
	1157.0	1156.7	0.3	0.02	5.93
	6058.0	6057.2	0.8	0.01	30.25
	5630.0	5630.2	-0.2	-0.00	28.18
	686.0	684.8	1.2	0.17	3.52
	559.0	557.5	1.5	0.27	2.87

0 440.411865 -141678.875000 0.001740

STANDARD DEVIATION OF CURVE-FITTING IS 3.01294994
AVERAGE O/O DEVIATION IS 0.07438529
NO.OF OBSERVATION = 12

0 440.411865 -141678.875000 0.001740

CALIBRATION TABLE FOR 5-JUNCTION COPPER CONSTNTAN THERMOPILE

	.0	.1	.2	.3	.4	.5	.6	.7	.8	.9	1.0	
0	0.	19.	39.	58.	78.	97.	116.	136.	155.	175.	194.	0
1	194.	214.	233.	252.	272.	291.	311.	330.	350.	369.	389.	1
2	389.	408.	428.	447.	466.	486.	505.	525.	544.	564.	583.	2
3	583.	603.	623.	642.	662.	681.	701.	720.	740.	759.	779.	3
4	779.	798.	818.	838.	857.	877.	896.	916.	936.	955.	975.	4
5	975.	994.	1014.	1033.	1053.	1073.	1092.	1112.	1132.	1151.	1171.	5
6	1171.	1191.	1210.	1230.	1249.	1269.	1289.	1308.	1328.	1348.	1368.	6
7	1368.	1387.	1407.	1427.	1446.	1466.	1486.	1505.	1525.	1545.	1565.	7
8	1565.	1584.	1604.	1624.	1644.	1663.	1683.	1703.	1723.	1742.	1762.	8
9	1762.	1782.	1802.	1821.	1841.	1861.	1881.	1901.	1920.	1940.	1960.	9
10	1960.	1980.	2000.	2019.	2039.	2059.	2079.	2099.	2119.	2138.	2158.	10
11	2158.	2178.	2198.	2218.	2238.	2258.	2277.	2297.	2317.	2337.	2357.	11
12	2357.	2377.	2397.	2417.	2437.	2457.	2476.	2496.	2516.	2536.	2556.	12
13	2556.	2576.	2596.	2616.	2636.	2656.	2676.	2696.	2716.	2736.	2756.	13
14	2756.	2776.	2796.	2816.	2836.	2856.	2876.	2896.	2916.	2936.	2956.	14
15	2956.	2976.	2996.	3016.	3036.	3056.	3076.	3096.	3116.	3136.	3156.	15
16	3156.	3176.	3196.	3216.	3236.	3257.	3277.	3297.	3317.	3337.	3357.	16
17	3357.	3377.	3397.	3417.	3437.	3458.	3478.	3498.	3518.	3538.	3558.	17
18	3558.	3578.	3599.	3619.	3639.	3659.	3679.	3699.	3720.	3740.	3760.	18
19	3760.	3780.	3800.	3821.	3841.	3861.	3881.	3901.	3922.	3942.	3962.	19
20	3962.	3982.	4003.	4023.	4043.	4063.	4084.	4104.	4124.	4144.	4155.	20
21	4165.	4185.	4205.	4225.	4246.	4266.	4286.	4307.	4327.	4347.	4368.	21
22	4368.	4388.	4408.	4428.	4449.	4469.	4489.	4510.	4530.	4550.	4571.	22
23	4571.	4591.	4612.	4632.	4652.	4673.	4693.	4713.	4734.	4754.	4775.	23
24	4775.	4795.	4815.	4836.	4856.	4877.	4897.	4917.	4938.	4958.	4979.	24

	.0	.1	.2	.3	.4	.5	.6	.7	.8	.9	1.0	
25	4979.	4999.	5020.	5040.	5060.	5081.	5101.	5122.	5142.	5163.	5183.	25
26	5183.	5204.	5224.	5245.	5265.	5286.	5306.	5327.	5347.	5368.	5388.	26
27	5388.	5409.	5429.	5450.	5470.	5491.	5511.	5532.	5552.	5573.	5594.	27
28	5594.	5614.	5635.	5655.	5676.	5696.	5717.	5738.	5758.	5779.	5799.	28
29	5799.	5820.	5841.	5861.	5882.	5902.	5923.	5944.	5964.	5985.	6006.	29
30	6006.	6026.	6047.	6068.	6088.	6109.	6130.	6150.	6171.	6192.	6212.	30
31	6212.	6233.	6254.	6274.	6295.	6316.	6336.	6357.	6378.	6399.	6419.	31
32	6419.	6440.	6461.	6481.	6502.	6523.	6544.	6564.	6585.	6606.	6627.	32
33	6627.	6647.	6668.	6689.	6710.	6731.	6751.	6772.	6793.	6814.	6834.	33
34	6834.	6855.	6876.	6897.	6918.	6939.	6959.	6980.	7001.	7022.	7043.	34
35	7043.	7064.	7084.	7105.	7126.	7147.	7168.	7189.	7210.	7231.	7251.	35
36	7251.	7272.	7293.	7314.	7335.	7356.	7377.	7398.	7419.	7440.	7460.	36
37	7460.	7481.	7502.	7523.	7544.	7565.	7586.	7607.	7628.	7649.	7670.	37
38	7670.	7691.	7712.	7733.	7754.	7775.	7796.	7817.	7838.	7859.	7880.	38
39	7880.	7901.	7922.	7943.	7964.	7985.	8006.	8027.	8048.	8069.	8090.	39
40	8090.	8111.	8132.	8153.	8174.	8195.	8216.	8237.	8258.	8279.	8301.	40
41	8300.	8322.	8343.	8364.	8385.	8406.	8427.	8448.	8469.	8490.	8512.	41
42	8512.	8533.	8554.	8575.	8596.	8617.	8638.	8660.	8681.	8702.	8723.	42
43	8723.	8744.	8765.	8787.	8808.	8829.	8850.	8871.	8892.	8914.	8935.	43
44	8935.	8956.	8977.	8998.	9020.	9041.	9062.	9083.	9105.	9126.	9147.	44
45	9147.	9168.	9190.	9211.	9232.	9253.	9275.	9296.	9317.	9338.	9360.	45
46	9360.	9381.	9402.	9424.	9445.	9466.	9488.	9509.	9530.	9551.	9573.	46
47	9573.	9594.	9615.	9637.	9658.	9679.	9701.	9722.	9744.	9765.	9786.	47
48	9786.	9807.	29.	9850.	9872.	9893.	9914.	9936.	9957.	9979.	10000.	48
49	10000.	10021.	10043.	10064.	10086.	10107.	10129.	10150.	10171.	10193.	10214.	49
50	10214.	10236.	10257.	10279.	10300.	10321.	10343.	10364.	10386.	10407.	10429.	50
51	10429.	10450.	10472.	10493.	10515.	10536.	10558.	10579.	10601.	10622.	10644.	51
52	10644.	10665.	10687.	10708.	10730.	10751.	10773.	10795.	10816.	10838.	10859.	52
53	10859.	10881.	10902.	10924.	10945.	10967.	10989.	11010.	11032.	11053.	11075.	53
54	11075.	11097.	11118.	11140.	11161.	11183.	11205.	11226.	11248.	11270.	11291.	54
55	11291.	11313.	11334.	11356.	11378.	11399.	11421.	11443.	11464.	11486.	11508.	55
56	11508.	11529.	11551.	11573.	11594.	11616.	11638.	11659.	11681.	11703.	11725.	56
							11812.	11833.	11855.	11877.	11898.	11920.	11942.	57

APPENDIX II

Calibration of the Pressure Gauge by Measuring Vapor Pressure of (i) Research Grade Benzene and Using Antoine Equation

Pressure Gauge Reading	t°C	$P = \text{Antilog } a - \frac{b}{t+c}$
6.001	6.68	38.19
6.124	7.02	38.90
7.123	9.88	45.28
7.185	10.07	45.73
7:732	1.43	49.08
8.285	12.80	52.66
8.565	13.47	54.49
9.366	15.29	59.73
10.039	16.63	63.85
10.704	17.97	68.20
11.830	20.00	75.26
1.867	20.07	75.52
13.212	22.34	84.14
15.009	25.05	95.48
15.177	25.32	96.67
(ii) Research Grade n-Hexane		
7.296	0.43	46.40
7.778	1.64	49.48
8.594	3.53	54.63
9.550	5.65	60.93
10.807	8.05	68.78
11.849	9.93	75.49
13.470	12.56	85.78
15.074	14.93	96.02
17.023	17.53	108.40
19.020	19.96	121.11
21.115	22.33	134.67
23.930	25.17	152.52

PROGRAM JP-2 (REV 12.3.1971)
PRESSURE GAUGE TABULATION,

GAUGE NO.1981,TUBE NO.4625,WATER EBULIO.MAR31,71

COEFFICIENTS:

A0 = 0.10708D-01 (+-) 0.14988D-01
A1 = 0.15707D 00 (+-) 0.37002D-03
A2 =-0.16832D-05 (+-) 0.20494D-05

P	GAUGE READING EXP	CALC	DIF
38.190	6.001	6.007	0.006
38.900	6.124	6.118	-0.006
45.280	7.123	7.119	-0.004
45.730	7.185	7.190	0.005
49.080	7.732	7.716	-0.017
52.660	8.285	8.277	-0.008
54.490	8.565	8.564	-0.001
59.730	9.366	9.387	0.020
63.850	10.039	10.033	-0.006
68.200	10.704	10.715	0.011
75.260	11.830	11.822	-0.008
75.520	11.867	11.863	-0.004
84.140	13.212	13.215	0.002
95.480	15.009	14.992	-0.017
96.670	15.177	15.179	0.002
46.400	7.296	7.295	-0.001
49.480	7.778	7.778	0.000
54.630	8.594	8.586	-0.008
60.930	9.550	9.575	0.025
68.780	10.807	10.806	-0.001
75.490	11.849	11.858	0.009
85.780	13.470	13.472	0.001
96.020	15.074	15.077	0.003
108.400	17.023	17.017	-0.006
121.110	19.020	19.009	-0.012
134.670	21.116	21.133	0.017
152.520	23.931	23.928	-0.003
		MEAN	0.010

P/G.R.	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.0	0.011	0.026	0.042	0.058	0.074	0.089	0.105	0.121	0.136	0.152	0.168
1.0	0.168	0.183	0.199	0.215	0.231	0.246	0.262	0.278	0.293	0.309	0.325
2.0	0.325	0.341	0.356	0.372	0.388	0.403	0.419	0.435	0.450	0.466	0.482
3.0	0.482	0.498	0.513	0.529	0.545	0.560	0.576	0.592	0.608	0.623	0.639
4.0	0.639	0.655	0.670	0.686	0.702	0.717	0.733	0.749	0.765	0.780	0.796
5.0	0.796	0.812	0.827	0.843	0.859	0.875	0.890	0.906	0.922	0.937	0.953
6.0	0.953	0.969	0.984	1.000	1.016	1.032	1.047	1.063	1.079	1.094	1.110
7.0	1.110	1.126	1.142	1.157	1.173	1.189	1.204	1.220	1.236	1.251	1.267
8.0	1.267	1.283	1.299	1.314	1.330	1.346	1.361	1.377	1.393	1.409	1.424
9.0	1.424	1.440	1.456	1.471	1.487	1.503	1.518	1.534	1.550	1.566	1.581
10.0	1.581	1.597	1.613	1.628	1.644	1.660	1.675	1.691	1.707	1.723	1.738
11.0	1.738	1.754	1.770	1.785	1.801	1.817	1.832	1.848	1.864	1.880	1.895
12.0	1.895	1.911	1.927	1.942	1.958	1.974	1.990	2.005	2.021	2.037	2.052
13.0	2.052	2.068	2.084	2.099	2.115	2.131	2.147	2.162	2.178	2.194	2.209
14.0	2.209	2.225	2.241	2.256	2.272	2.288	2.304	2.319	2.335	2.351	2.366
15.0	2.366	2.382	2.398	2.413	2.429	2.445	2.461	2.476	2.492	2.508	2.523
16.0	2.523	2.539	2.555	2.571	2.586	2.602	2.618	2.633	2.649	2.665	2.680
17.0	2.680	2.696	2.712	2.728	2.743	2.759	2.775	2.790	2.806	2.822	2.837
18.0	2.837	2.853	2.869	2.885	2.900	2.916	2.932	2.947	2.963	2.979	2.994
19.0	2.994	3.010	3.026	3.042	3.057	3.073	3.089	3.104	3.120	3.136	3.151
20.0	3.151	3.167	3.183	3.199	3.214	3.230	3.246	3.261	3.277	3.293	3.308
21.0	3.308	3.324	3.340	3.356	3.371	3.387	3.403	3.418	3.434	3.450	3.465
22.0	3.465	3.481	3.497	3.513	3.528	3.544	3.560	3.575	3.591	3.607	3.622
23.0	3.622	3.638	3.654	3.670	3.685	3.701	3.717	3.732	3.748	3.764	3.779
24.0	3.779	3.795	3.811	3.827	3.842	3.858	3.874	3.889	3.905	3.921	3.936
25.0	3.936	3.952	3.968	3.984	3.999	4.015	4.031	4.046	4.062	4.078	4.093
26.0	4.093	4.109	4.125	4.140	4.156	4.172	4.188	4.203	4.219	4.235	4.250
27.0	4.250	4.266	4.282	4.297	4.313	4.329	4.345	4.360	4.376	4.392	4.407
28.0	4.407	4.423	4.439	4.454	4.470	4.486	4.502	4.517	4.533	4.549	4.564
29.0	4.564	4.580	4.596	4.611	4.627	4.643	4.659	4.674	4.690	4.706	4.721
30.0	4.721	4.737	4.753	4.768	4.784	4.800	4.815	4.831	4.847	4.863	4.878
31.0	4.878	4.894	4.910	4.925	4.941	4.957	4.972	4.988	5.004	5.020	5.035
32.0	5.035	5.051	5.067	5.082	5.098	5.114	5.129	5.145	5.161	5.177	5.192
33.0	5.192	5.208	5.224	5.239	5.255	5.271	5.286	5.302	5.318	5.333	5.349
34.0	5.349	5.365	5.381	5.396	5.412	5.428	5.443	5.459	5.475	5.490	5.506

P/G.R.	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
35.0	5.506	5.522	5.538	5.553	5.569	5.585	5.600	5.616	5.632	5.647	5.663
36.0	5.663	5.679	5.694	5.710	5.726	5.742	5.757	5.773	5.789	5.804	5.820
37.0	5.820	5.836	5.851	5.867	5.883	5.898	5.914	5.930	5.946	5.961	5.977
38.0	5.977	5.993	6.008	6.024	6.040	6.055	6.071	6.087	6.103	6.118	6.134
39.0	6.134	6.150	6.165	6.181	6.197	6.212	6.228	6.244	6.259	6.275	6.291
40.0	6.291	6.307	6.322	6.338	6.354	6.369	6.385	6.401	6.416	6.432	6.448
41.0	6.448	6.463	6.479	6.495	6.511	6.526	6.542	6.558	6.573	6.589	6.605
42.0	6.605	6.620	6.636	6.652	6.667	6.683	6.699	6.715	6.730	6.746	6.762
43.0	6.762	6.777	6.793	6.809	6.824	6.840	6.856	6.871	6.887	6.903	6.919
44.0	6.919	6.934	6.950	6.966	6.981	6.997	7.013	7.028	7.044	7.060	7.075
45.0	7.075	7.091	7.107	7.123	7.138	7.154	7.170	7.185	7.201	7.217	7.232
46.0	7.232	7.248	7.264	7.279	7.295	7.311	7.327	7.342	7.358	7.374	7.389
47.0	7.389	7.405	7.421	7.436	7.452	7.468	7.483	7.499	7.515	7.531	7.546
48.0	7.546	7.562	7.578	7.593	7.609	7.625	7.640	7.656	7.672	7.687	7.703
49.0	7.703	7.719	7.735	7.750	7.766	7.782	7.797	7.813	7.829	7.844	7.860
50.0	7.860	7.876	7.891	7.907	7.923	7.938	7.954	7.970	7.986	8.001	8.017
51.0	8.017	8.033	8.048	8.064	8.080	8.095	8.111	8.127	8.142	8.158	8.174
52.0	8.174	8.190	8.205	8.221	8.237	8.252	8.268	8.284	8.299	8.315	8.331
53.0	8.331	8.346	8.362	8.378	8.393	8.409	8.425	8.441	8.456	8.472	8.488
54.0	8.488	8.503	8.519	8.535	8.550	8.566	8.582	8.597	8.613	8.629	8.644
55.0	8.644	8.660	8.676	8.692	8.707	8.723	8.739	8.754	8.770	8.786	8.801
56.0	8.801	8.817	8.833	8.848	8.864	8.880	8.896	8.911	8.927	8.943	8.958
57.0	8.958	8.974	8.990	9.005	9.021	9.037	9.052	9.068	9.084	9.099	9.115
58.0	9.115	9.131	9.147	9.162	9.178	9.194	9.209	9.225	9.241	9.256	9.272
59.0	9.272	9.288	9.303	9.319	9.335	9.350	9.366	9.382	9.398	9.413	9.429
60.0	9.429	9.445	9.460	9.476	9.492	9.507	9.523	9.539	9.554	9.570	9.586
61.0	9.586	9.601	9.617	9.633	9.648	9.664	9.680	9.696	9.711	9.727	9.743
62.0	9.743	9.758	9.774	9.790	9.805	9.821	9.837	9.852	9.868	9.884	9.899
63.0	9.899	9.915	9.931	9.947	9.962	9.978	9.994	10.009	10.025	10.041	10.056
64.0	10.056	10.072	10.088	10.103	10.119	10.135	10.150	10.166	10.182	10.197	10.213
65.0	10.213	10.229	10.245	10.260	10.276	10.292	10.307	10.323	10.339	10.354	10.370
66.0	10.370	10.386	10.401	10.417	10.433	10.448	10.464	10.480	10.496	10.511	10.527
67.0	10.527	10.543	10.558	10.574	10.590	10.605	10.621	10.637	10.652	10.668	10.684
68.0	10.684	10.699	10.715	10.731	10.746	10.762	10.778	10.794	10.809	10.825	10.841
69.0	10.841	10.856	10.872	10.888	10.903	10.919	10.935	10.950	10.966	10.982	10.997

P/G.P.	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
70.0	10.997	11.013	11.029	11.044	11.060	11.076	11.092	11.107	11.123	11.139	11.154
71.0	11.154	11.170	11.186	11.201	11.217	11.233	11.248	11.264	11.280	11.295	11.311
72.0	11.311	11.327	11.342	11.358	11.374	11.389	11.405	11.421	11.437	11.452	11.468
73.0	11.468	11.484	11.499	11.515	11.531	11.546	11.562	11.578	11.593	11.609	11.625
74.0	11.625	11.640	11.656	11.672	11.687	11.703	11.719	11.734	11.750	11.766	11.782
75.0	11.782	11.797	11.813	11.829	11.844	11.860	11.876	11.891	11.907	11.923	11.938
76.0	11.938	11.954	11.970	11.985	12.001	12.017	12.032	12.048	12.064	12.079	12.095
77.0	12.095	12.111	12.127	12.142	12.158	12.174	12.189	12.205	12.221	12.236	12.252
78.0	12.252	12.268	12.283	12.299	12.315	12.330	12.346	12.362	12.377	12.393	12.409
79.0	12.409	12.424	12.440	12.456	12.471	12.487	12.503	12.519	12.534	12.550	12.566
80.0	12.566	12.581	12.597	12.613	12.628	12.644	12.660	12.675	12.691	12.707	12.722
81.0	12.722	12.738	12.754	12.769	12.785	12.801	12.816	12.832	12.848	12.863	12.879
82.0	12.879	12.895	12.911	12.926	12.942	12.958	12.973	12.989	13.005	13.020	13.036
83.0	13.036	13.052	13.067	13.083	13.099	13.114	13.130	13.146	13.161	13.177	13.193
84.0	13.193	13.208	13.224	13.240	13.255	13.271	13.287	13.303	13.318	13.334	13.350
85.0	13.350	13.365	13.381	13.397	13.412	13.428	13.444	13.459	13.475	13.491	13.506
86.0	13.506	13.522	13.538	13.553	13.569	13.585	13.600	13.616	13.632	13.647	13.663
87.0	13.663	13.679	13.694	13.710	13.726	13.741	13.757	13.773	13.789	13.804	13.820
88.0	13.820	13.836	13.851	13.867	13.883	13.898	13.914	13.930	13.945	13.961	13.977
89.0	13.977	13.992	14.008	14.024	14.039	14.055	14.071	14.086	14.102	14.118	14.133
90.0	14.133	14.149	14.165	14.180	14.196	14.212	14.227	14.243	14.259	14.275	14.290
91.0	14.290	14.306	14.322	14.337	14.353	14.369	14.384	14.400	14.416	14.431	14.447
92.0	14.447	14.463	14.478	14.494	14.510	14.525	14.541	14.557	14.572	14.588	14.604
93.0	14.604	14.619	14.635	14.651	14.666	14.682	14.698	14.713	14.729	14.745	14.760
94.0	14.760	14.776	14.792	14.807	14.823	14.839	14.855	14.870	14.886	14.902	14.917
95.0	14.917	14.933	14.949	14.964	14.980	14.996	15.011	15.027	15.043	15.058	15.074
96.0	15.074	15.090	15.105	15.121	15.137	15.152	15.168	15.184	15.199	15.215	15.231
97.0	15.231	15.246	15.262	15.278	15.293	15.309	15.325	15.340	15.356	15.372	15.387
98.0	15.387	15.403	15.419	15.434	15.450	15.466	15.482	15.497	15.513	15.529	15.544
99.0	15.544	15.560	15.576	15.591	15.607	15.623	15.638	15.654	15.670	15.685	15.701
100.0	15.701	15.717	15.732	15.748	15.764	15.779	15.795	15.811	15.826	15.842	15.858
101.0	15.858	15.873	15.889	15.905	15.920	15.936	15.952	15.967	15.983	15.999	16.014
102.0	16.014	16.030	16.046	16.061	16.077	16.093	16.108	16.124	16.140	16.155	16.171
103.0	16.171	16.187	16.202	16.218	16.234	16.249	16.265	16.281	16.296	16.312	16.328
104.0	16.328	16.344	16.359	16.375	16.391	16.406	16.422	16.438	16.453	16.469	16.485

P/G.R.	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
105.0	16.485	16.500	16.516	16.532	16.547	16.563	16.579	16.594	16.610	16.626	16.641
106.0	16.641	16.657	16.673	16.688	16.704	16.720	16.735	16.751	16.767	16.782	16.798
107.0	16.798	16.814	16.829	16.845	16.861	16.876	16.892	16.908	16.923	16.939	16.955
108.0	16.955	16.970	16.986	17.002	17.017	17.033	17.049	17.064	17.080	17.096	17.111
109.0	17.111	17.127	17.143	17.158	17.174	17.190	17.205	17.221	17.237	17.252	17.268
110.0	17.268	17.284	17.299	17.315	17.331	17.346	17.362	17.378	17.393	17.409	17.425
111.0	17.425	17.440	17.456	17.472	17.487	17.503	17.519	17.534	17.550	17.566	17.581
112.0	17.581	17.597	17.613	17.629	17.644	17.660	17.676	17.691	17.707	17.723	17.738
113.0	17.738	17.754	17.770	17.785	17.801	17.817	17.832	17.848	17.864	17.879	17.895
114.0	17.895	17.911	17.926	17.942	17.958	17.973	17.989	18.005	18.020	18.036	18.052
115.0	18.052	18.067	18.083	18.099	18.114	18.130	18.146	18.161	18.177	18.193	18.208
116.0	18.208	18.224	18.240	18.255	18.271	18.287	18.302	18.318	18.334	18.349	18.365
117.0	18.365	18.381	18.396	18.412	18.428	18.443	18.459	18.475	18.490	18.506	18.522
118.0	18.522	18.537	18.553	18.569	18.584	18.600	18.616	18.631	18.647	18.663	18.678
119.0	18.678	18.694	18.710	18.725	18.741	18.757	18.772	18.788	18.804	18.819	18.835
120.0	18.835	18.851	18.866	18.882	18.898	18.913	18.929	18.945	18.960	18.976	18.992
121.0	18.992	19.007	19.023	19.039	19.054	19.070	19.086	19.101	19.117	19.133	19.148
122.0	19.148	19.164	19.180	19.195	19.211	19.227	19.242	19.258	19.274	19.289	19.305
123.0	19.305	19.321	19.336	19.352	19.368	19.383	19.399	19.415	19.430	19.446	19.462
124.0	19.462	19.477	19.493	19.509	19.524	19.540	19.556	19.571	19.587	19.603	19.618
125.0	19.618	19.634	19.650	19.665	19.681	19.697	19.712	19.728	19.744	19.759	19.775
126.0	19.775	19.791	19.806	19.822	19.838	19.853	19.869	19.885	19.900	19.916	19.932
127.0	19.932	19.947	19.963	19.979	19.994	20.010	20.026	20.041	20.057	20.072	20.088
128.0	20.088	20.104	20.119	20.135	20.151	20.166	20.182	20.198	20.213	20.229	20.245
129.0	20.245	20.260	20.276	20.292	20.307	20.323	20.339	20.354	20.370	20.386	20.401
130.0	20.401	20.417	20.433	20.448	20.464	20.480	20.495	20.511	20.527	20.542	20.558
131.0	20.558	20.574	20.589	20.605	20.621	20.636	20.652	20.668	20.683	20.699	20.715
132.0	20.715	20.730	20.746	20.762	20.777	20.793	20.809	20.824	20.840	20.856	20.871
133.0	20.871	20.887	20.903	20.918	20.934	20.950	20.965	20.981	20.997	21.012	21.028
134.0	21.028	21.044	21.059	21.075	21.091	21.106	21.122	21.138	21.153	21.169	21.185
135.0	21.185	21.200	21.216	21.232	21.247	21.263	21.279	21.294	21.310	21.326	21.341
136.0	21.341	21.357	21.372	21.388	21.404	21.419	21.435	21.451	21.466	21.482	21.498
137.0	21.498	21.513	21.529	21.545	21.560	21.576	21.592	21.607	21.623	21.639	21.654
138.0	21.654	21.670	21.686	21.701	21.717	21.733	21.748	21.764	21.780	21.795	21.811
139.0	21.811	21.827	21.842	21.858	21.874	21.889	21.905	21.921	21.936	21.952	21.968

P/G.R.	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
140.0	21.968	21.983	21.999	22.015	22.030	22.046	22.062	22.077	22.093	22.109	22.124
141.0	22.124	22.140	22.156	22.171	22.187	22.202	22.218	22.234	22.249	22.265	22.281
142.0	22.281	22.296	22.312	22.328	22.343	22.359	22.375	22.390	22.406	22.422	22.437
143.0	22.437	22.453	22.469	22.484	22.500	22.516	22.531	22.547	22.563	22.578	22.594
144.0	22.594	22.610	22.625	22.641	22.657	22.672	22.688	22.704	22.719	22.735	22.751
145.0	22.751	22.766	22.782	22.798	22.813	22.829	22.845	22.860	22.876	22.891	22.907
146.0	22.907	22.923	22.938	22.954	22.970	22.985	23.001	23.017	23.032	23.048	23.064
147.0	23.064	23.079	23.095	23.111	23.126	23.142	23.158	23.173	23.189	23.205	23.220
148.0	23.220	23.236	23.252	23.267	23.283	23.299	23.314	23.330	23.346	23.361	23.377
149.0	23.377	23.393	23.408	23.424	23.439	23.455	23.471	23.486	23.502	23.518	23.533
150.0	23.533	23.549	23.565	23.580	23.596	23.612	23.627	23.643	23.659	23.674	23.690
151.0	23.690	23.706	23.721	23.737	23.753	23.768	23.784	23.800	23.815	23.831	23.847
152.0	23.847	23.862	23.878	23.894	23.909	23.925	23.940	23.956	23.972	23.987	24.003
153.0	24.003	24.019	24.034	24.050	24.066	24.081	24.097	24.113	24.128	24.144	24.160
154.0	24.160	24.175	24.191	24.207	24.222	24.238	24.254	24.269	24.285	24.301	24.316
155.0	24.316	24.332	24.348	24.363	24.379	24.394	24.410	24.426	24.441	24.457	24.473
156.0	24.473	24.488	24.504	24.520	24.535	24.551	24.567	24.582	24.598	24.614	24.629
157.0	24.629	24.645	24.661	24.676	24.692	24.708	24.723	24.739	24.755	24.770	24.786
158.0	24.786	24.801	24.817	24.833	24.848	24.864	24.880	24.895	24.911	24.927	24.942
159.0	24.942	24.958	24.974	24.989	25.005	25.021	25.036	25.052	25.068	25.083	25.099
160.0	25.099	25.115	25.130	25.146	25.162	25.177	25.193	25.208	25.224	25.240	25.255
161.0	25.255	25.271	25.287	25.302	25.318	25.334	25.349	25.365	25.381	25.396	25.412
162.0	25.412	25.428	25.443	25.459	25.475	25.490	25.506	25.522	25.537	25.553	25.568
163.0	25.568	25.584	25.600	25.615	25.631	25.647	25.662	25.678	25.694	25.709	25.725
164.0	25.725	25.741	25.756	25.772	25.788	25.803	25.819	25.835	25.850	25.866	25.882
165.0	25.882	25.897	25.913	25.928	25.944	25.960	25.975	25.991	26.007	26.022	26.038
166.0	26.038	26.054	26.069	26.085	26.101	26.116	26.132	26.148	26.163	26.179	26.195
167.0	26.195	26.210	26.226	26.242	26.257	26.273	26.288	26.304	26.320	26.335	26.351
168.0	26.351	26.367	26.382	26.398	26.414	26.429	26.445	26.461	26.476	26.492	26.508
169.0	26.508	26.523	26.539	26.555	26.570	26.586	26.601	26.617	26.633	26.648	26.664
170.0	26.664	26.680	26.695	26.711	26.727	26.742	26.758	26.774	26.789	26.805	26.821
171.0	26.821	26.836	26.852	26.868	26.883	26.899	26.914	25.930	26.946	26.961	26.977
172.0	26.977	26.993	27.008	27.024	27.040	27.055	27.071	27.087	27.102	27.118	27.134
173.0	27.134	27.149	27.165	27.180	27.196	27.212	27.227	27.243	27.259	27.274	27.290
174.0	27.290	27.306	27.321	27.337	27.353	27.368	27.384	27.400	27.415	27.431	27.447

P/G.R.	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
175.0	27.447	27.462	27.478	27.493	27.509	27.525	27.540	27.556	27.572	27.587	27.603
176.0	27.603	27.619	27.634	27.650	27.666	27.681	27.697	27.713	27.728	27.744	27.759
177.0	27.759	27.775	27.791	27.806	27.822	27.838	27.853	27.869	27.885	27.900	27.916
178.0	27.916	27.932	27.947	27.963	27.979	27.994	28.010	28.025	28.041	28.057	28.072
179.0	28.072	28.088	28.104	28.119	28.135	28.151	28.166	28.182	28.198	28.213	28.229
180.0	28.229	28.245	28.260	28.276	28.291	28.307	28.323	28.338	28.354	28.370	28.385
181.0	28.385	28.401	28.417	28.432	28.448	28.464	28.479	28.495	28.511	28.526	28.542
182.0	28.542	28.557	28.573	28.589	28.604	28.620	28.636	28.651	28.667	28.683	28.698
183.0	28.698	28.714	28.730	28.745	28.761	28.776	28.792	28.808	28.823	28.839	28.855
184.0	28.855	28.870	28.886	28.902	28.917	28.933	28.949	28.964	28.980	28.996	29.011
185.0	29.011	29.027	29.042	29.058	29.074	29.089	29.105	29.121	29.136	29.152	29.168
186.0	29.168	29.183	29.199	29.215	29.230	29.246	29.261	29.277	29.293	29.308	29.324
187.0	29.324	29.340	29.355	29.371	29.387	29.402	29.418	29.434	29.449	29.465	29.480
188.0	29.480	29.496	29.512	29.527	29.543	29.559	29.574	29.590	29.606	29.621	29.637
189.0	29.637	29.653	29.668	29.684	29.699	29.715	29.731	29.746	29.762	29.778	29.793
190.0	29.793	29.809	29.825	29.840	29.856	29.872	29.887	29.903	29.918	29.934	29.950
191.0	29.950	29.965	29.981	29.997	30.012	30.028	30.044	30.059	30.075	30.091	30.106
192.0	30.106	30.122	30.137	30.153	30.169	30.184	30.200	30.216	30.231	30.247	30.263
193.0	30.263	30.278	30.294	30.310	30.325	30.341	30.356	30.372	30.388	30.403	30.419
194.0	30.419	30.435	30.450	30.466	30.482	30.497	30.513	30.529	30.544	30.560	30.575
195.0	30.575	30.591	30.607	30.622	30.638	30.654	30.669	30.685	30.701	30.716	30.732
196.0	30.732	30.748	30.763	30.779	30.794	30.810	30.826	30.841	30.857	30.873	30.888
197.0	30.888	30.904	30.920	30.935	30.951	30.966	30.982	30.998	31.013	31.029	31.045
198.0	31.045	31.060	31.076	31.092	31.107	31.123	31.139	31.154	31.170	31.185	31.201
199.0	31.201	31.217	31.232	31.248	31.264	31.279	31.295	31.311	31.326	31.342	31.357
200.0	31.357	31.373	31.389	31.404	31.420	31.436	31.451	31.467	31.483	31.498	31.514

APPENDIX III

Data for Mole Fraction Against Density

Cyclohexane-Benzene

x_1	Density *	V^E
0.0	0.87358	0.0
0.1391	0.85460	0.28019
0.2910	0.83602	0.49470
0.3847	0.82554	0.58193
0.5448	0.80946	0.61758
0.7537	0.79144	0.46388
0.8740	0.78249	0.26197
1.0	0.77385	0.0

n-Hexane-Cyclohexane

0.00	0.77385	0.0
0.1545	0.75196	0.04954
0.2191	0.74325	0.06497
0.3498	0.82640	0.08139
0.5195	0.70607	0.05190
0.6670	0.68957	0.00009
0.8070	0.67553	-0.01595
1.0	0.65480	0.00

n-Hexane-Benzene

0.0	0.87358	0.0
0.0855	0.84762	-0.05535
0.0855	0.84762	-0.02994
0.3086	0.78561	0.16009
0.4693	0.74785	0.29309
0.6267	0.71584	0.32230
0.7569	0.69264	0.23636
0.8642	0.67524	0.12386
1.0	0.65480	0.0

* K. Ridgway [2]

PROGRAM JP-28, MOL. FRACTION VS.DENSITY

BENZENE(1) - CYCLOHEXANE(2)
D(1) = 0.87384 D(2) = 0.77383 MW(1) = 78.108 MW(2) = 84.156
EXCESS VOLUME EQ. COEFFS:
C1 = 2.490700 C2 = 0.151801 C3 = -0.222473 C4 = -0.202182 C5 = 0.0 C6 = 0.0

X/D	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.0	0.77383	0.77390	0.77396	0.77403	0.77410	0.77416	0.77423	0.77430	0.77436	0.77443
0.01	0.77450	0.77456	0.77463	0.77470	0.77476	0.77483	0.77490	0.77496	0.77503	0.77510
0.02	0.77516	0.77523	0.77530	0.77537	0.77543	0.77550	0.77557	0.77563	0.77570	0.77577
0.03	0.77584	0.77590	0.77597	0.77604	0.77611	0.77617	0.77624	0.77631	0.77638	0.77644
0.04	0.77651	0.77658	0.77665	0.77671	0.77678	0.77685	0.77692	0.77699	0.77705	0.77712
0.05	0.77719	0.77726	0.77733	0.77739	0.77746	0.77753	0.77760	0.77767	0.77773	0.77780
0.06	0.77787	0.77794	0.77801	0.77808	0.77815	0.77821	0.77828	0.77835	0.77842	0.77849
0.07	0.77856	0.77863	0.77870	0.77876	0.77883	0.77890	0.77897	0.77904	0.77911	0.77918
0.08	0.77925	0.77932	0.77939	0.77946	0.77953	0.77960	0.77966	0.77973	0.77980	0.77987
0.09	0.77994	0.78001	0.78008	0.78015	0.78022	0.78029	0.78036	0.78043	0.78050	0.78057
0.10	0.78064	0.78071	0.78078	0.78085	0.78092	0.78099	0.78106	0.78113	0.78121	0.78128
0.11	0.78135	0.78142	0.78149	0.78156	0.78163	0.78170	0.78177	0.78184	0.78191	0.78198
0.12	0.78206	0.78213	0.78220	0.78227	0.78234	0.78241	0.78248	0.78255	0.78263	0.78270
0.13	0.78277	0.78284	0.78291	0.78298	0.78306	0.78313	0.78320	0.78327	0.78334	0.78342
0.14	0.78349	0.78356	0.78363	0.78371	0.78378	0.78385	0.78392	0.78400	0.78407	0.78414
0.15	0.78421	0.78429	0.78436	0.78443	0.78450	0.78458	0.78465	0.78472	0.78480	0.78487
0.16	0.78494	0.78502	0.78509	0.78516	0.78524	0.78531	0.78538	0.78545	0.78553	0.78561
0.17	0.78568	0.78575	0.78583	0.78590	0.78598	0.78605	0.78612	0.78620	0.78627	0.78635
0.18	0.78642	0.78650	0.78657	0.78664	0.78672	0.78679	0.78687	0.78694	0.78702	0.78709
0.19	0.78717	0.78724	0.78732	0.78739	0.78747	0.78754	0.78762	0.78770	0.78777	0.78785
0.20	0.78792	0.78800	0.78807	0.78815	0.78823	0.78830	0.78838	0.78845	0.78853	0.78861
0.21	0.78868	0.78876	0.78883	0.78891	0.78899	0.78906	0.78914	0.78922	0.78929	0.78937
0.22	0.78945	0.78953	0.78960	0.78968	0.78976	0.78983	0.78991	0.78999	0.79007	0.79014
0.23	0.79022	0.79030	0.79038	0.79045	0.79053	0.79061	0.79069	0.79077	0.79084	0.79092
0.24	0.79100	0.79108	0.79116	0.79124	0.79131	0.79139	0.79147	0.79155	0.79163	0.79171
0.25	0.79179	0.79186	0.79194	0.79202	0.79210	0.79218	0.79226	0.79234	0.79242	0.79250
0.26	0.79258	0.79266	0.79274	0.79282	0.79290	0.79298	0.79306	0.79314	0.79322	0.79330
0.27	0.79338	0.79346	0.79354	0.79362	0.79370	0.79378	0.79386	0.79394	0.79402	0.79410
0.28	0.79418	0.79427	0.79435	0.79443	0.79451	0.79459	0.79467	0.79475	0.79483	0.79492
0.29	0.79500	0.79508	0.79516	0.79524	0.79533	0.79541	0.79549	0.79557	0.79565	0.79574

PROGRAM JP-28, MOL. FRACTION VS. DENSITY

BENZENE(1) - CYCLOHEXANE(2)
D(1) = 0.87384 D(2) = 0.77383 MW(1) = 78.108 MW(2) = 84.156
EXCESS VOLUME EQ. COEFFS:
C1 = 2.490700 C2 = 0.151801 C3 = -0.222473 C4 = -0.202182 C5 = 0.0 C6 = 0.0

X/D	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.30	0.79582	0.79590	0.79598	0.79607	0.79615	0.79623	0.79631	0.79640	0.79648	0.79656
0.31	0.79665	0.79673	0.79681	0.79690	0.79698	0.79706	0.79715	0.79723	0.79731	0.79740
0.32	0.79748	0.79757	0.79765	0.79773	0.79782	0.79790	0.79799	0.79807	0.79815	0.79824
0.33	0.79832	0.79841	0.79849	0.79858	0.79866	0.79875	0.79883	0.79892	0.79900	0.79909
0.34	0.79917	0.79926	0.79934	0.79943	0.79952	0.79960	0.79969	0.79977	0.79986	0.79994
0.35	0.80003	0.80012	0.80020	0.80029	0.80038	0.80046	0.80055	0.80064	0.80072	0.80081
0.36	0.80090	0.80098	0.80107	0.80116	0.80124	0.80133	0.80142	0.80151	0.80159	0.80168
0.37	0.80177	0.80186	0.80194	0.80203	0.80212	0.80221	0.80230	0.80238	0.80247	0.80256
0.38	0.80265	0.80274	0.80283	0.80291	0.80300	0.80309	0.80318	0.80327	0.80336	0.80345
0.39	0.80354	0.80363	0.80372	0.80380	0.80389	0.80398	0.80407	0.80416	0.80425	0.80434
0.40	0.80443	0.80452	0.80461	0.80470	0.80479	0.80488	0.80497	0.80506	0.80516	0.80525
0.41	0.80534	0.80543	0.80552	0.80561	0.80570	0.80579	0.80588	0.80597	0.80607	0.80616
0.42	0.80625	0.80634	0.80643	0.80652	0.80662	0.80671	0.80680	0.80689	0.80698	0.80708
0.43	0.80717	0.80726	0.80735	0.80745	0.80754	0.80763	0.80772	0.80782	0.80791	0.80800
0.44	0.80810	0.80819	0.80828	0.80838	0.80847	0.80856	0.80866	0.80875	0.80884	0.80894
0.45	0.80903	0.80913	0.80922	0.80931	0.80941	0.80950	0.80960	0.80969	0.80979	0.80988
0.46	0.80998	0.81007	0.81016	0.81026	0.81035	0.81045	0.81055	0.81064	0.81074	0.81083
0.47	0.81093	0.81102	0.81112	0.81121	0.81131	0.81141	0.81150	0.81150	0.81169	0.81179
0.48	0.81189	0.81198	0.81208	0.81218	0.81227	0.81237	0.81247	0.81256	0.81266	0.81276
0.49	0.81286	0.81295	0.81305	0.81315	0.81324	0.81334	0.81344	0.81354	0.81364	0.81373
0.50	0.81383	0.81393	0.81403	0.81413	0.81422	0.81432	0.81442	0.81452	0.81462	0.81472
0.51	0.81482	0.81492	0.81501	0.81511	0.81521	0.81531	0.81541	0.81551	0.81561	0.81571
0.52	0.81581	0.81591	0.81601	0.81611	0.81621	0.81631	0.81641	0.81651	0.81661	0.81671
0.53	0.81681	0.81691	0.81701	0.81711	0.81721	0.81731	0.81742	0.81752	0.81762	0.81772
0.54	0.81782	0.81792	0.81802	0.81813	0.81823	0.81833	0.81843	0.81853	0.81863	0.81874
0.55	0.81884	0.81894	0.81904	0.81915	0.81925	0.81935	0.81945	0.81956	0.81966	0.81976
0.56	0.81987	0.81997	0.82007	0.82017	0.82028	0.82038	0.82049	0.82059	0.82069	0.82080
0.57	0.82090	0.82100	0.82111	0.82121	0.82132	0.82142	0.82152	0.82163	0.82173	0.82184
0.58	0.82194	0.82205	0.82215	0.82226	0.82236	0.82247	0.82257	0.82268	0.82278	0.82289
0.59	0.82300	0.82310	0.82321	0.82331	0.82342	0.82352	0.82363	0.82374	0.82384	0.82395

PROGRAM JP-28, MOL. FRACTION VS. DENSITY

BENZENE(1) - CYCLOHEXANE(2)
D(1) = 0.87384 D(2) = 0.77383 MW(1) = 78.108 MW(2) = 84.156
EXCESS VOLUME EQ. COEFFS:
C1 = 2.490700 C2 = 0.151801 C3 = -0.222473 C4 = -0.202182 C5 = 0.0 C6 = 0.0

X/D	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.60	0.82406	0.82416	0.82427	0.82437	0.82448	0.82459	0.82470	0.82480	0.82491	0.82502
0.61	0.82512	0.82523	0.82534	0.82545	0.82555	0.82566	0.82577	0.82588	0.82599	0.82609
0.62	0.82620	0.82631	0.82642	0.82653	0.82663	0.82674	0.82685	0.82696	0.82707	0.82718
0.63	0.82729	0.82740	0.82751	0.82761	0.82772	0.82783	0.82794	0.82805	0.82816	0.82827
0.64	0.82838	0.82849	0.82860	0.82871	0.82882	0.82893	0.82904	0.82915	0.82926	0.82937
0.65	0.82948	0.82960	0.82971	0.82982	0.82993	0.83004	0.83015	0.83026	0.83037	0.83048
0.66	0.83060	0.83071	0.83082	0.83093	0.83104	0.83115	0.83127	0.83138	0.83149	0.83160
0.67	0.83172	0.83183	0.83194	0.83205	0.83217	0.83228	0.83239	0.83251	0.83262	0.83273
0.68	0.83285	0.83296	0.83307	0.83319	0.83330	0.83341	0.83353	0.83364	0.83375	0.83387
0.69	0.83398	0.83410	0.83421	0.83433	0.83444	0.83455	0.83467	0.83478	0.83490	0.83501
0.70	0.83513	0.83524	0.83536	0.83547	0.83559	0.83571	0.83582	0.83594	0.83605	0.83617
0.71	0.83628	0.83640	0.83652	0.83663	0.83675	0.83686	0.83698	0.83710	0.83721	0.83733
0.72	0.83745	0.83756	0.83768	0.83780	0.83792	0.83803	0.83815	0.83827	0.83839	0.83850
0.73	0.83862	0.83874	0.83886	0.83897	0.83909	0.83921	0.83933	0.83945	0.83957	0.83968
0.74	0.83980	0.83992	0.84004	0.84016	0.84028	0.84040	0.84052	0.84063	0.84075	0.84087
0.75	0.84099	0.84111	0.84123	0.84135	0.84147	0.84159	0.84171	0.84183	0.84195	0.84207
0.76	0.84219	0.84231	0.84243	0.84255	0.84267	0.84280	0.84292	0.84304	0.84316	0.84328
0.77	0.84340	0.84352	0.84364	0.84376	0.84389	0.84401	0.84413	0.84425	0.84437	0.84450
0.78	0.84462	0.84474	0.84486	0.84499	0.84511	0.84523	0.84535	0.84548	0.84560	0.84572
0.79	0.84584	0.84597	0.84609	0.84621	0.84634	0.84646	0.84658	0.84671	0.84683	0.84696
0.80	0.84708	0.84720	0.84733	0.84745	0.84758	0.84770	0.84783	0.84795	0.84808	0.84820
0.81	0.84833	0.84845	0.84858	0.84870	0.84883	0.84895	0.84908	0.84920	0.84933	0.84945
0.82	0.84958	0.84971	0.84983	0.84996	0.85008	0.85021	0.85034	0.85046	0.85059	0.85072
0.83	0.85084	0.85097	0.85110	0.85122	0.85135	0.85148	0.85161	0.85173	0.85186	0.85199
0.84	0.85212	0.85224	0.85237	0.85250	0.85263	0.85276	0.85288	0.85301	0.85314	0.85327
0.85	0.85340	0.85353	0.85366	0.85378	0.85391	0.85404	0.85417	0.85430	0.85443	0.85456
0.86	0.85469	0.85482	0.85495	0.85508	0.85521	0.85534	0.85547	0.85560	0.85573	0.85586
0.87	0.85599	0.85612	0.85625	0.85638	0.85651	0.85665	0.85678	0.85691	0.85704	0.85717
0.88	0.85730	0.85743	0.85757	0.85770	0.85783	0.85796	0.85809	0.85823	0.85836	0.85849
0.89	0.85862	0.85876	0.85889	0.85902	0.85916	0.85929	0.85942	0.85955	0.85969	0.85982

PROGRAM JP-28, MOL. FRACTION VS. DENSITY

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EXCESS VOLUME EQ. COEFFS:
C1 = 2.490700 C2 = 0.151801 C3 = -0.222473 C4 = -0.202182 C5 = 0.0 C6 = 0.0

X/D	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.90	0.85996	0.86009	0.86022	0.86036	0.86049	0.86062	0.86076	0.86089	0.86103	0.86116
0.91	0.86130	0.86143	0.86157	0.86170	0.86184	0.86197	0.86211	0.86224	0.86238	0.86251
0.92	0.86265	0.86278	0.86292	0.86305	0.86319	0.86333	0.86346	0.86360	0.86374	0.86387
0.93	0.86401	0.86415	0.86428	0.86442	0.86456	0.86469	0.86483	0.86497	0.86511	0.86524
0.94	0.86538	0.86552	0.86566	0.86579	0.86593	0.86607	0.86621	0.86635	0.86649	0.86662
0.95	0.86676	0.86690	0.86704	0.86718	0.86732	0.86746	0.86760	0.86774	0.86788	0.86802
0.96	0.86816	0.86830	0.86844	0.86858	0.86872	0.86886	0.86900	0.86914	0.86928	0.86942
0.97	0.86956	0.86970	0.86984	0.86998	0.87013	0.87027	0.87041	0.87055	0.87069	0.87083
0.98	0.87098	0.87112	0.87126	0.87140	0.87155	0.87169	0.87183	0.87197	0.87212	0.87226
0.99	0.87240	0.87255	0.87269	0.87283	0.87298	0.87312	0.87326	0.87341	0.87355	0.87370
1.00	0.87384	0.87398	0.87413	0.87427	0.87442	0.87456	0.87471	0.87485	0.87500	0.87514

PROGRAM JP-28, MOL. FRACTION VS.DENSITY

N-HEXANE(1) - CYCLOHEXANE(2)
D(1) = 0.65490 D(2) = 0.77383 MW(1) = 86.172 MW(2) = 84.156
EXCESS VOLUME EQ. COEFFS:
C1 = 0.217732 C2 = 0.588105 C3 = -0.214599 C4 = -0.487134 C5 = 0.0 C6 = 0.0

X/D	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.0	0.77383	0.77369	0.77354	0.77340	0.77325	0.77311	0.77296	0.77282	0.77267	0.77253
0.01	0.77238	0.77224	0.77210	0.77195	0.77181	0.77165	0.77152	0.77138	0.77123	0.77109
0.02	0.77094	0.77080	0.77065	0.77051	0.77037	0.77022	0.77008	0.76994	0.76979	0.76965
0.03	0.76950	0.76936	0.76922	0.76907	0.76893	0.76879	0.76864	0.76850	0.76836	0.76821
0.04	0.76807	0.76793	0.76778	0.76764	0.76750	0.76735	0.76721	0.76707	0.76692	0.76678
0.05	0.76664	0.76649	0.76635	0.76621	0.76607	0.76592	0.76578	0.76564	0.76550	0.76535
0.06	0.76521	0.76507	0.76493	0.76478	0.76464	0.76450	0.75436	0.76421	0.76407	0.76393
0.07	0.76379	0.76365	0.76350	0.76336	0.76322	0.76308	0.76294	0.76280	0.76265	0.76251
0.08	0.76237	0.76223	0.76209	0.76195	0.76181	0.76166	0.76152	0.76138	0.76124	0.76110
0.09	0.76096	0.76082	0.76068	0.76054	0.76039	0.76025	0.75011	0.75997	0.75983	0.75969
0.10	0.75955	0.75941	0.75927	0.75913	0.75899	0.75885	0.75871	0.75857	0.75843	0.75829
0.11	0.75815	0.75801	0.75787	0.75773	0.75759	0.75745	0.75731	0.75717	0.75703	0.75689
0.12	0.75675	0.75661	0.75647	0.75633	0.75620	0.75606	0.75592	0.75578	0.75564	0.75550
0.13	0.75536	0.75522	0.75508	0.75495	0.75481	0.75467	0.75453	0.75439	0.75425	0.75412
0.14	0.75398	0.75384	0.75370	0.75356	0.75343	0.75329	0.75315	0.75301	0.75287	0.75274
0.15	0.75260	0.75246	0.75232	0.75219	0.75205	0.75191	0.75178	0.75164	0.75150	0.75136
0.16	0.75123	0.75109	0.75095	0.75082	0.75068	0.75054	0.75041	0.75027	0.75013	0.75000
0.17	0.74986	0.74972	0.74959	0.74945	0.74932	0.74918	0.74904	0.74891	0.74877	0.74864
0.18	0.74850	0.74837	0.74823	0.74809	0.74795	0.74782	0.74769	0.74755	0.74742	0.74728
0.19	0.74715	0.74701	0.74688	0.74674	0.74661	0.74647	0.74634	0.74621	0.74607	0.74594
0.20	0.74580	0.74567	0.74553	0.74540	0.74527	0.74513	0.74500	0.74486	0.74473	0.74460
0.21	0.74446	0.74433	0.74419	0.74406	0.74393	0.74379	0.74366	0.74353	0.74339	0.74326
0.22	0.74313	0.74300	0.74286	0.74273	0.74260	0.74246	0.74233	0.74220	0.74207	0.74193
0.23	0.74180	0.74167	0.74154	0.74141	0.74127	0.74114	0.74101	0.74088	0.74075	0.74061
0.24	0.74048	0.74035	0.74022	0.74009	0.73996	0.73982	0.73969	0.73956	0.73943	0.73930
0.25	0.73917	0.73904	0.73891	0.73878	0.73865	0.73852	0.73838	0.73825	0.73812	0.73799
0.26	0.73786	0.73773	0.73760	0.73747	0.73734	0.73721	0.73708	0.73695	0.73682	0.73669
0.27	0.73656	0.73643	0.73630	0.73617	0.73604	0.73592	0.73579	0.73566	0.73553	0.73540
0.28	0.73527	0.73514	0.73501	0.73488	0.73475	0.73463	0.73450	0.73437	0.73424	0.73411
0.29	0.73398	0.73385	0.73373	0.73360	0.73347	0.73334	0.73321	0.73309	0.73296	0.73283

PROGRAM JP-28, MOL. FRACTION VS. DENSITY

N-HEXANE(1) - CYCLOHEXANE(2)
D(1) = 0.65490 D(2) = 0.77383 MW(1) = 86.172 MW(2) = 84.156
EXCESS VOLUME EQ. COEFFS:
C1 = 0.217732 C2 = 0.588105 C3 = -0.214599 C4 = -0.487134 C5 = 0.0 C6 = 0.0

X/D	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.30	0.73270	0.73258	0.73245	0.73232	0.73219	0.73207	0.73194	0.73181	0.73168	0.73156
0.31	0.73143	0.73130	0.73118	0.73105	0.73092	0.73080	0.73067	0.73054	0.73042	0.73029
0.32	0.73016	0.73004	0.72991	0.72978	0.72966	0.72953	0.72941	0.72928	0.72915	0.72903
0.33	0.72890	0.72878	0.72865	0.72853	0.72840	0.72828	0.72815	0.72802	0.72790	0.72777
0.34	0.72765	0.72752	0.72740	0.72727	0.72715	0.72702	0.72690	0.72678	0.72665	0.72653
0.35	0.72640	0.72628	0.72615	0.72603	0.72590	0.72578	0.72566	0.72553	0.72541	0.72528
0.36	0.72516	0.72504	0.72491	0.72479	0.72467	0.72454	0.72442	0.72430	0.72417	0.72405
0.37	0.72393	0.72380	0.72368	0.72356	0.72343	0.72331	0.72319	0.72306	0.72294	0.72282
0.38	0.72270	0.72257	0.72245	0.72233	0.72221	0.72208	0.72196	0.72184	0.72172	0.72160
0.39	0.72147	0.72135	0.72123	0.72111	0.72099	0.72086	0.72074	0.72062	0.72050	0.72038
0.40	0.72026	0.72014	0.72001	0.71989	0.71977	0.71965	0.71953	0.71941	0.71929	0.71917
0.41	0.71905	0.71893	0.71880	0.71868	0.71855	0.71844	0.71832	0.71820	0.71808	0.71796
0.42	0.71784	0.71772	0.71760	0.71748	0.71736	0.71724	0.71712	0.71700	0.71688	0.71676
0.43	0.71664	0.71652	0.71640	0.71628	0.71616	0.71604	0.71592	0.71581	0.71569	0.71557
0.44	0.71545	0.71533	0.71521	0.71509	0.71497	0.71485	0.71473	0.71462	0.71450	0.71438
0.45	0.71426	0.71414	0.71402	0.71390	0.71379	0.71367	0.71355	0.71343	0.71331	0.71319
0.46	0.71308	0.71296	0.71284	0.71272	0.71260	0.71249	0.71237	0.71225	0.71213	0.71202
0.47	0.71190	0.71178	0.71166	0.71155	0.71143	0.71131	0.71119	0.71108	0.71096	0.71084
0.48	0.71073	0.71061	0.71049	0.71038	0.71026	0.71014	0.71002	0.70991	0.70979	0.70967
0.49	0.70956	0.70944	0.70933	0.70921	0.70909	0.70898	0.70886	0.70874	0.70863	0.70851
0.50	0.70840	0.70828	0.70816	0.70805	0.70793	0.70782	0.70770	0.70759	0.70747	0.70735
0.51	0.70724	0.70712	0.70701	0.70689	0.70678	0.70666	0.70655	0.70643	0.70632	0.70620
0.52	0.70609	0.70597	0.70586	0.70574	0.70563	0.70551	0.70540	0.70528	0.70517	0.70505
0.53	0.70494	0.70482	0.70471	0.70459	0.70448	0.70436	0.70425	0.70414	0.70402	0.70391
0.54	0.70379	0.70368	0.70357	0.70345	0.70334	0.70322	0.70311	0.70300	0.70288	0.70277
0.55	0.70265	0.70254	0.70243	0.70231	0.70220	0.70209	0.70197	0.70186	0.70175	0.70163
0.56	0.70152	0.70141	0.70129	0.70118	0.70107	0.70095	0.70084	0.70073	0.70061	0.70050
0.57	0.70039	0.70028	0.70016	0.70005	0.69994	0.69982	0.69971	0.69960	0.69949	0.69937
0.58	0.69926	0.69915	0.69904	0.69892	0.69881	0.69870	0.69859	0.69848	0.69836	0.69825
0.59	0.69814	0.69803	0.69792	0.69780	0.69769	0.69758	0.69747	0.69736	0.69724	0.69713

PROGRAM JP-28, MOL. FRACTION VS. DENSITY

N-HEXANE(1) - CYCLOHEXANE(2)
D(1) = 0.65490 D(2) = 0.77383 MW(1) = 86.172 MW(2) = 84.156
EXCESS VOLUME EQ. COEFFS:
C1 = 0.217732 C2 = 0.588105 C3 = -0.214599 C4 = -0.487134 C5 = 0.0 C6 = 0.0

X/D	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.60	0.69702	0.69691	0.69680	0.69669	0.69657	0.69646	0.69635	0.69624	0.69613	0.69602
0.61	0.69591	0.69579	0.69568	0.69557	0.69546	0.69535	0.69524	0.69513	0.69502	0.69491
0.62	0.69479	0.69468	0.69457	0.69446	0.69435	0.69424	0.69413	0.69402	0.69391	0.69380
0.63	0.69369	0.69358	0.69347	0.69336	0.69325	0.69313	0.69302	0.69291	0.69280	0.69269
0.64	0.69258	0.69247	0.69236	0.69225	0.69214	0.69203	0.69192	0.69181	0.69170	0.69159
0.65	0.69148	0.69137	0.69126	0.69115	0.69104	0.69093	0.69082	0.69072	0.69061	0.69050
0.66	0.69039	0.69028	0.69017	0.69006	0.68995	0.68984	0.68973	0.68962	0.68951	0.68940
0.67	0.68929	0.68918	0.68907	0.68897	0.68886	0.68875	0.68864	0.68853	0.68842	0.68831
0.68	0.68820	0.68809	0.68799	0.68788	0.68777	0.68766	0.68755	0.68744	0.68733	0.68722
0.69	0.68712	0.68701	0.68690	0.68679	0.68668	0.68657	0.68647	0.68636	0.68625	0.68614
0.70	0.68603	0.68592	0.68582	0.68571	0.68560	0.68549	0.68538	0.68528	0.68517	0.68506
0.71	0.68495	0.68484	0.68474	0.68463	0.68452	0.68441	0.68430	0.68420	0.68409	0.68398
0.72	0.68387	0.68377	0.68366	0.68355	0.68344	0.68334	0.68323	0.68312	0.68301	0.68291
0.73	0.68280	0.68269	0.68258	0.68248	0.68237	0.68226	0.68216	0.68205	0.68194	0.68183
0.74	0.68173	0.68162	0.68151	0.68141	0.68130	0.68119	0.68109	0.68098	0.68087	0.68077
0.75	0.68066	0.68055	0.68045	0.68034	0.68023	0.68013	0.68002	0.67991	0.67981	0.67970
0.76	0.67959	0.67949	0.67938	0.67927	0.67917	0.67906	0.67895	0.67885	0.67874	0.67864
0.77	0.67853	0.67842	0.67832	0.67821	0.67811	0.67800	0.67789	0.67779	0.67768	0.67758
0.78	0.67747	0.67736	0.67726	0.67715	0.67705	0.67694	0.67683	0.67673	0.67662	0.67652
0.79	0.67641	0.67631	0.67620	0.67610	0.67599	0.67588	0.67578	0.67567	0.67557	0.67546
0.80	0.67536	0.67525	0.67515	0.67504	0.67494	0.67483	0.67473	0.67462	0.67452	0.67441
0.81	0.67431	0.67420	0.67410	0.67399	0.67389	0.67378	0.67368	0.67357	0.67347	0.67336
0.82	0.67326	0.67315	0.67305	0.67294	0.67284	0.67273	0.67263	0.67252	0.67242	0.67231
0.83	0.67221	0.67211	0.67200	0.67190	0.67179	0.67169	0.67158	0.67148	0.67138	0.67127
0.84	0.67117	0.67106	0.67096	0.67085	0.67075	0.67065	0.67054	0.67044	0.67033	0.67023
0.85	0.67013	0.67002	0.66992	0.66981	0.66971	0.66961	0.66950	0.66940	0.66930	0.66919
0.86	0.66909	0.66899	0.66888	0.66878	0.66867	0.66857	0.66847	0.66836	0.66826	0.66816
0.87	0.66805	0.66795	0.66785	0.66774	0.66764	0.66754	0.66743	0.66733	0.66723	0.66713
0.88	0.66702	0.66692	0.66682	0.66671	0.66661	0.66651	0.66641	0.66630	0.66620	0.66610
0.89	0.66599	0.66589	0.66579	0.66569	0.66558	0.66548	0.66538	0.66528	0.66517	0.66507

PROGRAM JP-28, MOL. FRACTION VS. DENSITY

N-HEXANE(1) - CYCLOHEXANE(2)
D(1) = 0.65490 D(2) = 0.77383 MW(1) = 86.172 MW(2) = 84.156
EXCESS VOLUME EQ. COEFFS:
C1 = 0.217732 C2 = 0.588105 C3 = -0.214599 C4 = -0.487134 C5 = 0.0 C6 = 0.0

X/D	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.90	0.66497	0.66487	0.66476	0.66466	0.66456	0.66445	0.66435	0.66425	0.66415	0.66405
0.91	0.66395	0.66384	0.66374	0.66364	0.66354	0.66344	0.66333	0.66323	0.66313	0.66303
0.92	0.66293	0.66282	0.66272	0.66262	0.66252	0.66242	0.66232	0.66222	0.66211	0.66201
0.93	0.66191	0.66181	0.66171	0.66161	0.66151	0.66140	0.66130	0.66120	0.66110	0.66100
0.94	0.66090	0.66080	0.66070	0.66060	0.66049	0.66039	0.66029	0.66019	0.66009	0.65999
0.95	0.65989	0.65979	0.65969	0.65959	0.65949	0.65939	0.65929	0.65918	0.65908	0.65898
0.96	0.65888	0.65878	0.65868	0.65858	0.65848	0.65838	0.65828	0.65818	0.65808	0.65798
0.97	0.65788	0.65778	0.65768	0.65758	0.65748	0.65738	0.65728	0.65718	0.65708	0.65698
0.98	0.65688	0.65678	0.65668	0.65659	0.65649	0.65639	0.65629	0.65619	0.65609	0.65599
0.99	0.65589	0.65579	0.65569	0.65559	0.65549	0.65539	0.65530	0.65520	0.65510	0.65500
1.00	0.65490	0.65480	0.65470	0.65460	0.65451	0.65441	0.65431	0.65421	0.65411	0.65401

PROGRAM JP-28, MOL. FRACTION VS.DENSITY

N-HEXANE(1) - BENZENE(2)
D(1) = 0.65490 D(2) = 0.87384 MW(1) = 86.172 MW(2) = 78.108
EXCESS VOLUME EQ. COEFFS:
C1 = 1.267920 C2 = -0.993370 C3 = -1.855060 C4 = 0.0 C5 = 0.0 C6 = 0.0

X/D	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.0	0.87384	0.87353	0.87323	0.87292	0.87261	0.87231	0.87200	0.87169	0.87139	0.87108
0.01	0.87077	0.87047	0.87016	0.86986	0.86955	0.86925	0.86894	0.86863	0.86833	0.86802
0.02	0.86772	0.86741	0.86711	0.86680	0.86650	0.86619	0.86589	0.86558	0.86528	0.86497
0.03	0.86467	0.86436	0.86406	0.86376	0.86345	0.86315	0.86284	0.86254	0.86224	0.86193
0.04	0.86163	0.86133	0.86102	0.86072	0.86042	0.86011	0.85981	0.85951	0.85920	0.85890
0.05	0.85860	0.85830	0.85800	0.85769	0.85739	0.85709	0.85679	0.85649	0.85618	0.85588
0.06	0.85558	0.85528	0.85498	0.85468	0.85438	0.85408	0.85378	0.85348	0.85318	0.85288
0.07	0.85258	0.85228	0.85198	0.85168	0.85138	0.85108	0.85078	0.85048	0.85018	0.84988
0.08	0.84958	0.84929	0.84899	0.84869	0.84839	0.84809	0.84780	0.84750	0.84720	0.84690
0.09	0.84661	0.84631	0.84601	0.84572	0.84542	0.84512	0.84483	0.84453	0.84423	0.84394
0.10	0.84364	0.84335	0.84305	0.84276	0.84246	0.84217	0.84187	0.84158	0.84128	0.84099
0.11	0.84069	0.84040	0.84011	0.83981	0.83952	0.83923	0.83893	0.83864	0.83835	0.83805
0.12	0.83776	0.83747	0.83718	0.83688	0.83659	0.83630	0.83601	0.83572	0.83543	0.83514
0.13	0.83485	0.83455	0.83426	0.83397	0.83368	0.83339	0.83310	0.83281	0.83252	0.83223
0.14	0.83195	0.83166	0.83137	0.83108	0.83079	0.83050	0.83021	0.82993	0.82964	0.82935
0.15	0.82906	0.82878	0.82849	0.82820	0.82792	0.82763	0.82734	0.82706	0.82677	0.82649
0.16	0.82620	0.82592	0.82563	0.82535	0.82506	0.82478	0.82449	0.82421	0.82392	0.82364
0.17	0.82336	0.82307	0.82279	0.82251	0.82222	0.82194	0.82166	0.82138	0.82109	0.82081
0.18	0.82053	0.82025	0.81997	0.81969	0.81940	0.81912	0.81884	0.81856	0.81828	0.81800
0.19	0.81772	0.81744	0.81716	0.81689	0.81661	0.81633	0.81605	0.81577	0.81549	0.81521
0.20	0.81494	0.81466	0.81438	0.81410	0.81383	0.81355	0.81327	0.81300	0.81272	0.81245
0.21	0.81217	0.81189	0.81162	0.81134	0.81107	0.81079	0.81052	0.81025	0.80997	0.80970
0.22	0.80942	0.80915	0.80888	0.80860	0.80833	0.80806	0.80779	0.80751	0.80724	0.80697
0.23	0.80670	0.80643	0.80616	0.80588	0.80561	0.80534	0.80507	0.80480	0.80453	0.80426
0.24	0.80399	0.80372	0.80345	0.80319	0.80292	0.80265	0.80238	0.80211	0.80184	0.80158
0.25	0.80131	0.80104	0.80078	0.80051	0.80024	0.79998	0.79971	0.79944	0.79918	0.79891
0.26	0.79865	0.79838	0.79812	0.79785	0.79759	0.79732	0.79706	0.79680	0.79653	0.79627
0.27	0.79601	0.79574	0.79548	0.79522	0.79496	0.79469	0.79443	0.79417	0.79391	0.79365
0.28	0.79339	0.79313	0.79287	0.79261	0.79235	0.79209	0.79183	0.79157	0.79131	0.79105
0.29	0.79079	0.79053	0.79027	0.79002	0.78976	0.78950	0.78924	0.78899	0.78873	0.78847

PROGRAM JP-28, MOL. FRACTION VS. DENSITY

N-HEXANE(1) - BENZENE(2)
D(1) = 0.65490 D(2) = 0.87384 MW(1) = 86.172 MW(2) = 78.108
EXCESS VOLUME EQ. COEFFS:
C1 = 1.267920 C2 = -0.993370 C3 = -1.855060 C4 = 0.0 C5 = 0.0 C6 = 0.0

X/D	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.30	0.78822	0.78796	0.78770	0.78745	0.78719	0.78694	0.78668	0.78643	0.78617	0.78592
0.31	0.78566	0.78541	0.78515	0.78490	0.78465	0.78439	0.78414	0.78389	0.78364	0.78338
0.32	0.78313	0.78288	0.78263	0.78238	0.78213	0.78187	0.78162	0.78137	0.78112	0.78087
0.33	0.78062	0.78037	0.78012	0.77987	0.77963	0.77938	0.77913	0.77888	0.77863	0.77838
0.34	0.77814	0.77789	0.77764	0.77739	0.77715	0.77690	0.77665	0.77641	0.77616	0.77592
0.35	0.77567	0.77543	0.77518	0.77494	0.77469	0.77445	0.77420	0.77396	0.77372	0.77347
0.36	0.77323	0.77299	0.77274	0.77250	0.77226	0.77202	0.77177	0.77153	0.77129	0.77105
0.37	0.77081	0.77057	0.77033	0.77009	0.76985	0.76961	0.76937	0.76913	0.76889	0.76865
0.38	0.76841	0.76817	0.76793	0.76770	0.76746	0.76722	0.76698	0.76675	0.76651	0.76627
0.39	0.76604	0.76580	0.76556	0.76533	0.76509	0.76486	0.76462	0.76439	0.76415	0.76392
0.40	0.76368	0.76345	0.76321	0.76298	0.76275	0.76251	0.76228	0.76205	0.76182	0.76158
0.41	0.76135	0.76112	0.76089	0.76066	0.76042	0.76019	0.75996	0.75973	0.75950	0.75927
0.42	0.75904	0.75881	0.75858	0.75835	0.75812	0.75789	0.75767	0.75744	0.75721	0.75698
0.43	0.75675	0.75653	0.75630	0.75607	0.75584	0.75562	0.75539	0.75517	0.75494	0.75471
0.44	0.75449	0.75426	0.75404	0.75381	0.75359	0.75336	0.75314	0.75291	0.75269	0.75247
0.45	0.75224	0.75202	0.75180	0.75157	0.75135	0.75113	0.75091	0.75068	0.75046	0.75024
0.46	0.75002	0.74980	0.74958	0.74936	0.74914	0.74892	0.74870	0.74848	0.74826	0.74804
0.47	0.74782	0.74760	0.74738	0.74716	0.74694	0.74673	0.74651	0.74629	0.74607	0.74585
0.48	0.74564	0.74542	0.74520	0.74499	0.74477	0.74455	0.74434	0.74412	0.74391	0.74369
0.49	0.74348	0.74326	0.74305	0.74283	0.74262	0.74241	0.74219	0.74198	0.74176	0.74155
0.50	0.74134	0.74113	0.74091	0.74070	0.74049	0.74028	0.74007	0.73985	0.73964	0.73943
0.51	0.73922	0.73901	0.73880	0.73859	0.73838	0.73817	0.73796	0.73775	0.73754	0.73733
0.52	0.73712	0.73691	0.73671	0.73650	0.73629	0.73608	0.73587	0.73567	0.73546	0.73525
0.53	0.73504	0.73484	0.73463	0.73442	0.73422	0.73401	0.73381	0.73360	0.73340	0.73319
0.54	0.73299	0.73278	0.73258	0.73237	0.73217	0.73196	0.73176	0.73156	0.73135	0.73115
0.55	0.73095	0.73075	0.73054	0.73034	0.73014	0.72994	0.72973	0.72953	0.72933	0.72913
0.56	0.72893	0.72873	0.72853	0.72833	0.72813	0.72793	0.72773	0.72753	0.72733	0.72713
0.57	0.72693	0.72673	0.72653	0.72633	0.72614	0.72594	0.72574	0.72554	0.72534	0.72515
0.58	0.72495	0.72475	0.72456	0.72436	0.72416	0.72397	0.72377	0.72357	0.72338	0.72318
0.59	0.72299	0.72279	0.72260	0.72240	0.72221	0.72201	0.72182	0.72163	0.72143	0.72124

PROGRAM JP-28, MOL. FRACTION VS.DENSITY

N-HEXANE(1) - BENZENE(2)
D(1) = 0.65490 D(2) = 0.87384 MW(1) = 86.172 MW(2) = 78.108
EXCESS VOLUME EQ. COEFFS:
C1 = 1.267920 C2 = -0.993370 C3 = -1.855060 C4 = 0.0 C5 = 0.0 C6 = 0.0

X/D	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.60	0.72105	0.72085	0.72066	0.72047	0.72027	0.72008	0.71989	0.71970	0.71950	0.71931
0.61	0.71912	0.71893	0.71874	0.71855	0.71836	0.71816	0.71797	0.71778	0.71759	0.71740
0.62	0.71721	0.71702	0.71683	0.71664	0.71646	0.71627	0.71608	0.71589	0.71570	0.71551
0.63	0.71532	0.71514	0.71495	0.71476	0.71457	0.71439	0.71420	0.71401	0.71383	0.71364
0.64	0.71345	0.71327	0.71308	0.71289	0.71271	0.71252	0.71234	0.71215	0.71197	0.71178
0.65	0.71160	0.71141	0.71123	0.71104	0.71086	0.71068	0.71049	0.71031	0.71013	0.70994
0.66	0.70976	0.70958	0.70939	0.70921	0.70903	0.70885	0.70857	0.70848	0.70830	0.70812
0.67	0.70794	0.70776	0.70758	0.70740	0.70721	0.70703	0.70685	0.70667	0.70649	0.70631
0.68	0.70613	0.70595	0.70577	0.70560	0.70542	0.70524	0.70506	0.70488	0.70470	0.70452
0.69	0.70434	0.70417	0.70399	0.70381	0.70363	0.70346	0.70328	0.70310	0.70292	0.70275
0.70	0.70257	0.70239	0.70222	0.70204	0.70187	0.70169	0.70151	0.70134	0.70116	0.70099
0.71	0.70081	0.70064	0.70046	0.70029	0.70011	0.69994	0.69976	0.69959	0.69942	0.69924
0.72	0.69907	0.69890	0.69872	0.69855	0.69838	0.69820	0.69803	0.69786	0.69768	0.69751
0.73	0.69734	0.69717	0.69700	0.69682	0.69665	0.69648	0.69631	0.69614	0.69597	0.69580
0.74	0.69563	0.69545	0.69528	0.69511	0.69494	0.69477	0.69460	0.69443	0.69426	0.69409
0.75	0.69392	0.69376	0.69359	0.69342	0.69325	0.69308	0.69291	0.69274	0.69257	0.69241
0.76	0.69224	0.69207	0.69190	0.69173	0.69157	0.69140	0.69123	0.69105	0.69090	0.69073
0.77	0.69056	0.69040	0.69023	0.69006	0.68990	0.68973	0.68957	0.68940	0.68923	0.68907
0.78	0.68890	0.68874	0.68857	0.68841	0.68824	0.68808	0.68791	0.68775	0.68758	0.68742
0.79	0.68725	0.68709	0.68693	0.68676	0.68660	0.68644	0.68627	0.68611	0.68595	0.68578
0.80	0.68562	0.68546	0.68529	0.68513	0.68497	0.68481	0.68464	0.68448	0.68432	0.68416
0.81	0.68399	0.68383	0.68367	0.68351	0.68335	0.68319	0.68303	0.68286	0.68270	0.68254
0.82	0.68238	0.68222	0.68206	0.68190	0.68174	0.68158	0.68142	0.68126	0.68110	0.68094
0.83	0.68078	0.68062	0.68046	0.68030	0.68014	0.67998	0.67982	0.67957	0.67951	0.67935
0.84	0.67919	0.67903	0.67887	0.67871	0.67856	0.67840	0.67824	0.67808	0.67792	0.67777
0.85	0.67761	0.67745	0.67729	0.67714	0.67698	0.67682	0.67667	0.67651	0.67635	0.67620
0.86	0.67604	0.67588	0.67573	0.67557	0.67541	0.67526	0.67510	0.67495	0.67479	0.67463
0.87	0.67448	0.67432	0.67417	0.67401	0.67386	0.67370	0.67355	0.67339	0.67324	0.67308
0.88	0.67293	0.67277	0.67262	0.67246	0.67231	0.67216	0.67200	0.67185	0.67169	0.67154
0.89	0.67139	0.67123	0.67108	0.67092	0.67077	0.67062	0.67046	0.67031	0.67016	0.67000

PROGRAM JP-28, MOL. FRACTION VS.DENSITY

N-HEXANE(1) - BENZENE(2)
D(1) = 0.65490 D(2) = 0.87384 MW(1) = 86.172 MW(2) = 78.108
EXCESS VOLUME EQ. COEFFS:
C1 = 1.267920 C2 = -0.993370 C3 = -1.855060 C4 = 0.0 C5 = 0.0 C6 = 0.0

X/D	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.90	0.66985	0.66970	0.66955	0.66939	0.66924	0.66909	0.66894	0.66878	0.66863	0.66848
0.91	0.66833	0.66817	0.66802	0.66787	0.66772	0.66757	0.66741	0.66726	0.66711	0.66696
0.92	0.66681	0.66666	0.66651	0.66635	0.66620	0.66605	0.66590	0.66575	0.66560	0.66545
0.93	0.66530	0.66515	0.66500	0.66485	0.66470	0.66455	0.66439	0.66424	0.66409	0.66394
0.94	0.66379	0.66364	0.66349	0.66334	0.66319	0.66305	0.66290	0.66275	0.66260	0.66245
0.95	0.66230	0.66215	0.66200	0.66185	0.66170	0.66155	0.66140	0.66125	0.66110	0.66096
0.96	0.66081	0.66066	0.66051	0.66036	0.66021	0.66006	0.65992	0.65977	0.65962	0.65947
0.97	0.65932	0.65917	0.65903	0.65888	0.65873	0.65858	0.65843	0.65829	0.65814	0.65799
0.98	0.65784	0.65770	0.65755	0.65740	0.65725	0.65711	0.65696	0.65681	0.65666	0.65652
0.99	0.65637	0.65622	0.65608	0.65593	0.65578	0.65563	0.65549	0.65534	0.65519	0.65505
1.00	0.65490	0.65475	0.65461	0.65446	0.65431	0.65417	0.65402	0.65387	0.65373	0.65358

APPENDIX IV

COMPUTER PROGRAM FOR THE EVALUATION OF THE ANTOINE EQUATION CONSTANTS

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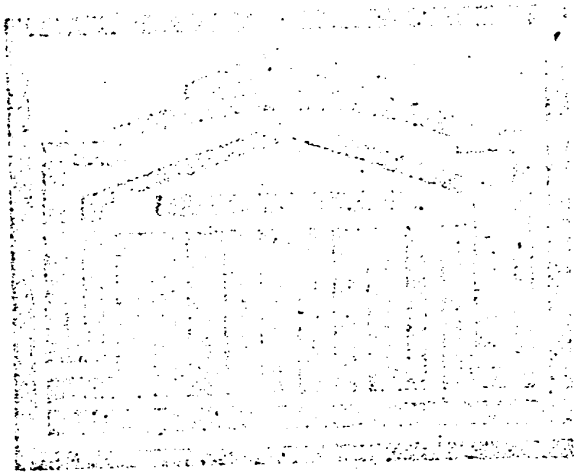
      C   PROGRAM  JP-3A (REV. 24.5.1972)
      C          DEPARTMENT OF CHEM. ENG., UNIVERSITY OF OTTAWA
      C   ANTOINE VAPOR PRESSURE CONSTANTS                                  80
0001      IMPLICIT REAL*8(A-H,O-Z)                                          90
0002      DIMENSION P(50),T(50),AA(3,4),SOL(3),F(4),KK(3),TITLE(20),W(50)   95
0003      DIMENSION  ERRSOL(3)                                              100
0004    100 READ (1,1000,END=115) TITLE                                     101
0005      READ (1,1140) NOMP,KCONST,KLIC,KTAB                               105
0006      IF (KTAB.NE.1.AND.KCONST.NE.1) GO TO 110                          106
0007      READ (1,1120) TEPL1, TEPL2                                        107
0008      IF (KCONST.NE.1) GO TO 110                                        108
0009      READ (1,1010) A,B,C                                               109
0010      GO TO 630                                                         110
0011    110 IF (NOMP.GT.0) GO TO 130                                        115
0012    115 WRITE (3,1070)                                                  120
0013      CALL EXIT                                                         130
0014    130 READ (1,1120) (T(K),P(K),K=1,NOMP)                              140
0015      A=DFLOAT(NOMP)/2.0D0+0.50000000100                                150
0016      KK(1)=1                                                           160
0017      KK(2)=IDINT(A)                                                    170
0018      KK(3)=NOMP                                                        180
0019      DO 220 L=1,3                                                      185
0020      N=KK(L)                                                           190
0021      AA(L,1)=T(N)                                                      200
0022      AA(L,2)=1                                                         210
0023      AA(L,3)=DLOG10(P(N))                                              220
0024    220 AA(L,4)=T(N)*AA(L,3)                                            222
0025      IF (KLIC.NE.1) GO TO 230                                          224
0026      WRITE (3,1150)                                                    226
0027      DO 224 L=1,3                                                      228
0028    224 WRITE (3,1160) (AA(L,K),K=1,4)
0029    230 CALL SCLVD (AA,3,3,4,0.D0,DET,TEST)                             231
0030      DO 232 K=1,3                                                      232
0031    232 SOL(K)=AA(K,4)                                                  240
0032      AO=SOL(1)                                                         250
0033      BO=SOL(2)                                                         26
0034      CO= SOL(3)                                                        265
0035      IF (KLIC.EQ.1) GO TO 830                                          270
0036    270 ALFA=0.000006D0                                                 280
0037      BETA=0.004D0                                                      290
0038      GAMA=0.004D0                                                      300
0039      DO 570 MM=1,20                                                    330
0040    330 DO 350 I=1,3
```

```
                                                                      340
0041            DO 350 J=1,4                                          350
0042        350 AA(I,J)=0.0                                           360
0043            DO 490 I=1,NOMP                                       370
0044            F(1)=T(I)                                             380
0045            F(2)=1.D0                                             390
0046            F(3)=DLOG10(P(I))                                     41
0047            F(4)=-(A0*T(I)+B0+C0*DLOG10(P(I))-T(I)*DLOG10(P(I)))  42
0048            E1=(ALFA+A0-DLOG10(P(I)))**2                          43
0049            E2=(GAMA+C0-T(I))**2                                  440
0050            SGT=9.0D-06                                           45
0051            SGLP=(0.03D0/(2.302585D0*P(I)))**2                    460
0052            W(I)=1.0D0 / (E1*SGT+E2*SGLP)                         470
0053            DO 490 J=1,3                                          480
0054            DO 490 K=J,4                                          490
0055        490 AA(J,K)=AA(J,K)+W(I)*F(J)*F(K)                        500
0056            DO 530 J=2,3                                          510
0057            L=J-1                                                 520
0058            DO 530 K=1,L                                          530
0059        530 AA(J,K)=AA(K,J)                                       531
0060            IF (KLIC.NE.1) GO TO 540                              532
0061            WRITE (3,1150)                                        533
0062            DO 534 L=1,3                                          534
0063        534 WRITE (3,1160) (AA(L,K),K=1,4)
0064        540 CALL SOLVD (AA,3,3,4,0.D0,DET,TEST)                   541
0065            DO 542 K=1,3                                          541A
0066            ERRSOL(K)=AA(K,K)                                     542
0067        542 SOL(K)=AA(K,4)                                        545
0068            IF (KLIC.EQ.1) GO TO 770                              546
0069            GO TO 880                                             770
0070        770 B1=A0+SOL(1)                                          780
0071            B2=B0+SOL(2)                                          790
0072            B3=C0+SOL(3)                                          800
0073            B2=-(B1*B3+B2)                                        810
0074            B3=-B3                                                820
0075            WRITE (3,1050) B1,B2,B3                               880
0076        880 B1=DABS(ALFA-SOL(1))                                  890
0077            B2=DABS(BETA-SOL(2))                                  900
0078            B3=DABS(GAMA-SOL(3))                                  91 10
0079            IF (B1-0.000003D0) 920,920,550                        910
0080        920 IF (B2-0.002D0) 930,930,550                           930
0081        930 IF (B3-0.02D0) 580,580,550                            550
0082        550 ALFA=SOL(1)                                           560
0083            BETA=SOL(2)
```

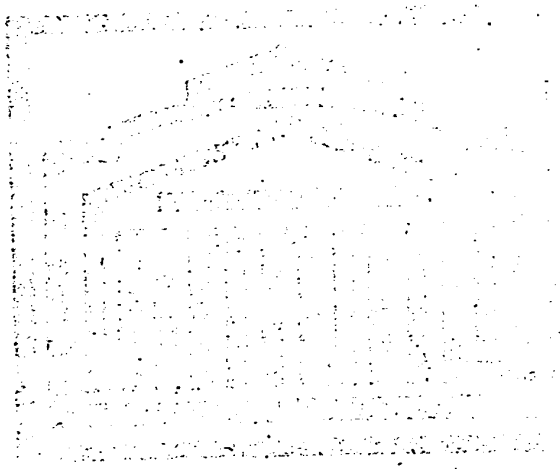
```
0084          570 GAMA=SCL(3)                                                   570
0085          580 A=AO+SCL(1)                                                   580
0086              B=BO+SOL(2)                                                   590
0087              C=CO+SOL(3)                                                   600
0088              B=-(A*C+B)                                                    610
0089              C=-C                                                          615
0090              SM=0.0                                                        621
0091              DO 624 K=1,NCMP                                               622
0092              PCL=DEXP(2.302585D0*(A-B/(T(K)+C)))                           623
0093          624 SM=SM+(PCL-P(K))**2*W(K)                                      624
0094              SM=DSQRT(SM/(NOMP-3))                                         625
0095              DO 627 K=1,3                                                  626
0096          627 ERRSOL(K)=SM*DSQRT(ERRSOL(K))                                 627
0097          630 CALL HEAD                                                     630
0098              WRITE (3,1020) TITLE, A,ERRSOL(1),B,ERRSOL(2),C,ERRSOL(3)     640
0099              IF (KCONST.NE.1) GO TO 650                                    641
0100              WRITE (3,1130)                                                642
0101              GO TO 960                                                     643
0102          650 SUM=0.0D0                                                     650
0103              SM=0.0                                                        655
0104              DO 700 K=1,NCMP                                               660
0105              PC=DEXP(2.302585D0*(A-B/(T(K)+C)))                            670
0106              DEV=PC-P(K)                                                   680
0107              DVP=DEV/P(K)*100.D0                                           684
0108              SM=SM+DVP*DVP                                                 688
0109              WRITE(3,1030) T(K),P(K),PC,DEV,DVP                            69
0110              IF (KLIC.EQ.1) WRITE (3,1060) W(K)                            695
0111          700 SUM=SUM+DEV*DEV                                               700
0112              S=DSQRT (SUM/(NOMP-3))                                        710
0113              SM=DSQRT(SM/(NOMP-3))                                         715
0114              WRITE (3,1040) S ,SM                                          720
0115              IF (KTAB.EQ.1) GO TO 960                                      940
0116              GO TO 100                                                     950
0117          960 N1=0                                                          960
0118              N2=35                                                         980
0119          990 IF (N2-35) 2030,2000,2000                                     990
0120         2000 WRITE (3,1050) TITLE,A,          B,C                        2000
0121              N2=0                                                         2010
0122              N1=0                                                         2020
0123         2030 IF (N1.LT.5) GO TO 2070                                      2030
0124              WRITE (3,1100)                                               2040
0125              N1=0                                                         2050
0126              N2=N2+1                                                      2060
```

```
0127          2070 DO 2090 K=1,11                                                    2070
0128               TT=TEPL1+(K-1)*0.1                                                2080
0129          2090 P(K)=DEXP (2.302585*(A-B/(TT+C)))                                 2090
0130               WRITE (3,1110) TEPL1,(P(K),K=1,11)                                2100
0131               TEPL1=TEPL1+1.0                                                   2110
0132               N1=N1+1                                                           2120
0133               N2=N2+1                                                           2130
0134               IF (TEPL2-TEPL1) 100,990,990                                      2140
0135          1000 FORMAT (20A4)                                                     100
0136          1010 FORMAT (3F10.5)                                                   1010
0137          1020 FORMAT (2X,20A4   ,///'  A =',F9.6,1X,'(+-)',F10.6,               1020.0
                  1/,'  B =',F9.3,' (+-)',F9.3,/,'  C =',F9.3,' (+-)',F9.3,///,T6,  1020=01
                  1'T', T14,'P EXP',T23,'P CALC',T33,'DEV',5X,'DEV%',//)            1020+1
0138          1030 FORMAT (1X,F6.3,2F10.3,F8.3,F8.2)                                 1030
0139          1040 FORMAT (/,1X,T23,'ST.DEV.',F8.3,F8.2)                             1050
0140          1050 FORMAT (3D16.7)                                                   1060
0141          1060 FORMAT ('+',T49,D12.4)                                            1070
0142          1070 FORMAT ('1',10X,'END OF JOB')                                     1090+0
0143          1090 FORMAT ('1',2X,20A4,//3X'ANTOINE VAPOR PRESSURE CONSTANTS'   ,    1090+1
                  1                                  / T8,'A =',F10.6,              1090+2
                  2/T8,'B =',F10.3,/T8,'C =',F10.3//3X,'T/P      0.0      0.1      0. 1090+3
                  32      0.3      0.4      0.5      0.6      0.7      0.8      0.9  1090+4
                  4    1.0'/)                                                       1100
0144          1100 FORMAT (3X)                                                       1110
0145          1110 FORMAT (1X,F6.1,11F9.2)                                           1120
0146          1120 FORMAT (2F10.5)                                                   1130+0
0147          1130 FORMAT (//3X'TABULATION OF THE VAPOR PRESSURE FROM THE GIVEN CONST 1130+1
                  1ANTS')                                                          1140
0148          1140 FORMAT (I2,2X,I1,5X,I1,9X,I1)                                     1150
0149          1150 FORMAT (3X,'NORMAL EQUATION MATRIX'/)                             1160
0150          1160 FORMAT (4D12.5)                                                   860
0151           830 WRITE (3,1050) A0,B0,C0                                           870
0152               GO TO 270                                                         MAIN
0153               END
```

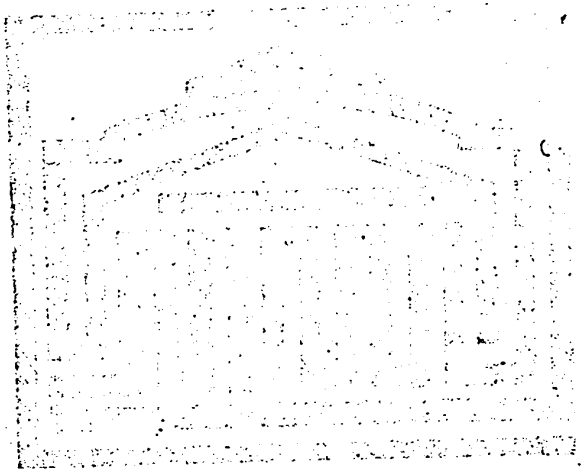
```
0001          SUBROUTINE HEAD                                                    10
0002          IMPLICIT REAL*8(T)                                                 20
0003          WRITE (3,1000)                                                     30
0004          RETURN
0005     1000 FORMAT('1',/,'  PROGRAM JP-3A (REV.24.5.1972). OUTPUT J.POLAK, DEP 1000+0
             1T.OF CHEM.ENG., UNIVERSITY OF OTTAWA',///,'  ANTOINE VAPOR PRESSUR 1000+1
             2E CONSTANTS',//)                                                  1000+2
0006          END                                                                HEAD
```



```
0001          SUBROUTINE SOLVD (X,IX,M,N,PREC,DET,TEST)                          SOLVD 1
0002          INTEGER*2 I1(255), I2(255)                                         SOLVD 2
0003          REAL*8 X(IX,N),T,DET,BIG,PREC,TEST,PIV,TEMP,DSQRT,DABS             SOLVD 3
0004          EQUIVALENCE (BIG,TEMP,PIV)                                         SOLVD 4
0005          DET=1.0D0                                                          SOLVD 5
0006          TEMP=DABS(PREC)                                                    SOLVD 6
0007          IF(TEMP.EQ.0.0D0) TEMP=0.5D-14                                     SOLVD 7
0008          TEST=0.D0                                                          SOLVD 8
0009          DO 1 I=1,M                                                         SOLVD 9
0010          I2(I)=0                                                            SOLVD10
0011          DO 1 J=1,M                                                         SOLVD11
0012        1 TEST=TEST+X(I,J)*X(I,J)                                            SOLVD12
0013          TEST=TEMP*DSQRT(TEST)/M                                            SOLVD13
0014          DO 9 K=1,M                                                         SOLVD14
0015          BIG=0.D0                                                           SOLVD15
0016          DO 3 I=1,M                                                         SOLVD16
0017          IF (I2(I).NE.0) GO TO 3                                            SOLVD17
0018          DO 2 J=1,M                                                         SOLVD18
0019          IF (I2(J).NE.0) GO TO 2                                            SOLVD19
0020          T=DABS(X(I,J))                                                     SOLVD20
0021          IF (T.LE.BIG) GO TO 2                                              SOLVD21
0022          BIG=T                                                              SOLVD22
0023          IROW=I                                                             SOLVD23
0024          JCOL=J                                                             SOLVD24
0025        2 CONTINUE                                                           SOLVD25
0026        3 CONTINUE                                                           SOLVD26
0027          IF (BIG.LE.TEST) RETURN                                            SOLVD27
0028          I1(K)=JCOL                                                         SOLVD28
0029          I2(JCOL)=IROW                                                      SOLVD29
0030          IF(JCOL.EQ.IROW) GO TO 6                                           SOLVD30
0031          DO 5 J=1,N                                                         SOLVD31
0032          TEMP=X(IROW,J)                                                     SOLVD32
0033          X(IROW,J)=X(JCOL,J)                                                SOLVD33
0034        5 X(JCOL,J)=TEMP                                                     SOLVD34
0035          DET=-DET                                                           SOLVD35
0036        6 DET=DET*X(JCOL,JCOL)                                               SOLVD36
0037          PIV=1.D0/X(JCOL,JCOL)                                              SOLVD37
0038          DO 7 J=1,N                                                         SOLVD38
0039          IF (J.NE.JCOL) X(JCOL,J)=PIV*X(JCOL,J)                             SOLVD39
0040        7 CONTINUE                                                           SOLVD40
0041          X(JCOL,JCOL)=PIV                                                   SOLVD41
0042          DO 9 I=1,M                                                         SOLVD42
0043          IF (I.EQ.JCOL) GO TO 9                                             SOLVD43
```



```
0044          PIV=-X(I,JCOL)                                                    SOLVD44
CC45          DC 8 J=1,N                                                        SOLVD45
0046          IF (J.NE.JCOL) X(I,J)=X(I,J)+PIV*X(JCCL,J)                        SOLVD46
0047        8 CCNTINUE                                                          SOLVD47
CC4E          X(I,JCCL)=PIV*X(JCCL,JCOL)                                        SOLVD48
0049        9 CONTINUE                                                          SOLVD49
0050          CO 11 K=1,M                                                       SOLVD50
CC51          I=M+1-K                                                           SOLVD51
0052          JCCL=I1(I)                                                        SOLVD52
0053          IROW=I2(JCOL)                                                     SOLVD53
CC54          IF(IROW.EQ.JCCL) GO TO 11                                         SOLVD54
0055          DO 10 I=1,M                                                       SOLVD55
0056          TEMP=X(I,IROW)                                                    SOLVD56
CC57          X(I,IROW)=X(I,JCCL)                                               SOLVD57
0058       10 X(I,JCCL)=TEMP                                                    SOLVD58
0059       11 CCNTINUE                                                          SOLVD59
CC60          TEST=0.CO                                                         SOLVD60
0061          RETURN                                                            SOLVD61
CC62          END                                                               SOLVD**
```



APPENDIX V

COMPUTER PROGRAM FOR THE EVALUATION OF THE TOTAL VAPOR PRESSURE CORRELATION CONSTANTS

```
      COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=45,SIZE=0000K,
                         SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,NOID,NOXREF
            C   JP-40 BINARY AND TERNARY TOTAL PRESSURE FIT,        DEPT OF CHEM,ENG.,U OF O
            C   PROGRAM NEW 26,5,1972
ISN 0002              IMPLICIT REAL*8(A-H,O-Z)
ISN 0003              DIMENSION TITLE(10),Y1(150),Y2(150),SOL(10),ERR(10),XWOBB(10)
ISN 0004              DIMENSION XMIMAX(10),PMIMAX(10),PWOBB(10)
ISN 0005              COMMON X1(150),X2(150),P(150),CC(3,8),P10,P20,P30,NCOMP,NCBIN,N2
ISN 0006              COMMON ILIMIT
ISN 0007              EXTERNAL FCE,FW,FREG,FSECD
ISN 0008           10 READ(1,1000) TITLE
ISN 0009              READ(1,1010) NCOMP,NCBIN,ICHECK,IPX,ILIMIT,TEMP,P10,P20,P30
ISN 0010              IF (NCOMP.EQ.0) CALL EXIT
ISN 0012              IF (NCOMP.EQ.3) GO TO 30
ISN 0014              DO 20 K=1,150
ISN 0015              READ(1,1020) X1(K),Y1(K),P(K)
ISN 0016              IF (IPX.EQ.1) P(K)=Y1(K)
ISN 0018              IF (X1(K).LT.0.0) GO TO 60
ISN 0020           20 CONTINUE
ISN 0021              GO TO 60
ISN 0022           30 DO 40 K=1,3
ISN 0023           40 READ(1,1020)(CC(K,I),I=1,8)
ISN 0024              DO 50 K=1,150
ISN 0025              READ(1,1020) X1(K), X2(K),Y1(K),Y2(K),P(K)
ISN 0026              IF (X1(K).EQ.0.0) GO TO 60
ISN 0028           50 CONTINUE
ISN 0029           60 NOMP=K-1
ISN 0030              DO 110 N1=1,NCBIN
ISN 0031              N2=N1
ISN 0032              IF (ILIMIT.EQ.1) N2=N2+2
ISN 0034              IF (ILIMIT.EQ.1.AND.N2.GE.NOMP) GO TO 10
ISN 0036              IF (NCOMP.EQ.3) N2=3
ISN 0038              CALL SQLIN(N2,NOMP,FCE,FW,SOL,ERR,0,0)
ISN 0039              WRITE(3,1030)
ISN 0040              IF (NCOMP.EQ.3) GOT O 100
ISN 0042              WRITE(3,1040) TITLE,TEMP,P10,P20
ISN 0043              DO 70 K=1,N2
ISN 0044              CC(1,K)=SOL(K)
ISN 0045           70 WRITE(3,1050) K,SOL(K),ERR(K)
ISN 0046              IF (ILIMIT.EQ.1) WRITE(3,1200)
ISN 0048              WRITE(3,1060)
ISN 0049              SD=0.0
ISN 0050              SDP=0.0
```

```
ISN 0051            DO 90 K=1,NOMP
ISN 0052            PC=PCALC(X1(K))
ISN 0053            DV=PC-P(K)
ISN 0054            DVP=DV/P(K)*100.D0
ISN 0055            WRITE(3,1070) X1(K),P(K),PC,DV,DVP
ISN 0056            SD=SD+DV*DV
ISN 0057         90 SDP=SDP+DVP*DVP
ISN 0058            SD=DSQRT(SD/(NOMP-N2))
ISN 0059            SDP=DSQRT(SDP/(NOMP-N2))
ISN 0060            WRITE(3,1080) SD,SDP
                 C   WOBBLING TEST
ISN 0061            XX1=0.0
ISN 0062            NWOBB=0
ISN 0063            NMIMAX=0
ISN 0064            DO 155 K=1,199
ISN 0065            XY1=XX1
ISN 0066            XZ1=XX1
ISN 0067            XX2=XX1+0.005D0
ISN 0068            CALL REGULA (FREG,XZ1,XX2,0.0001D0,ITER)
ISN 0069            IF (ITER.EQ.0) GO TO 150
ISN 0071            NMIMAX=NMIMAX+1
ISN 0072            XMIMAX(NMIMAX)=XZ1
ISN 0073            PMIMAX(NMIMAX)=PCALC(XZ1)
ISN 0074            GO TO 155
ISN 0075        150 CALL REGULA (FSECD,XY1,XX2,0.0001D0,ITER)
ISN 0076            IF(ITER.EQ.0) GO TO 155
ISN 0078            NWOBB=NWOBB+1
ISN 0079            XWOBB(NWOBB)=XY1
ISN 0080            PWOBB(NWOBB)=PCALC(XY1)
ISN 0081        155 XX1=XX2
ISN 0082            IF (NMIMAX.GT.0) GO TO 160
ISN 0084            IF (NWOBB.GT.0) GO TO 182
ISN 0086            WRITE(3,1160)
ISN 0087            GO TO 110
ISN 0088        160 DO 180 L=1,NMIMAX
ISN 0089            X=XMIMAX(L)
ISN 0090            S1=FSECD(X,I)
ISN 0091            IF (S1.LT.0.0) WRITE(3,1170) X,PMIMAX(L)
ISN 0093            IF (S1.GT.0.0) WRITE(3,1180) X,PMIMAX(L)
ISN 0095        180 CONTINUE
ISN 0096        182 IF (NWOBB.EQ.0) GO TO 110
ISN 0098            DO 185 L=1,NWOBB
ISN 0099        185 WRITE(3,1190) XWOBB(L),PWOBB(L)
```

```
ISN 0100        110 CONTINUE
ISN 0101            GO TO 10
ISN 0102        100 WRITE(3,1090)
ISN 0103            WRITE(3,1095) TITLE,TEMP,P10,P20,P30
ISN 0104            DO 145 MM=1,2
ISN 0105            IF (MM.EQ.1) GO TO 125
ISN 0107            DO 122 MN=1,3
ISN 0108            SOL(MN)=0.0
ISN 0109        122 ERR(MN)=0.0
ISN 0110        125 WRITE(3,1100) (I,I=1,6)
ISN 0111            K=NCBIN+1
ISN 0112            DO 120 I=1,3
ISN 0113        120 WRITE(3,1110) I,(CC(I,J),J=1,6)
ISN 0114            WRITE(3,1120) (SOL(I),ERR(I),I=1,3)
ISN 0115            WRITE(3,1130)
ISN 0116            S=0.0
ISN 0117            SP=0.0
ISN 0118            DO 140 K=1,NOMP
ISN 0119            X3=1.D0-X1(K)-X2(K)
ISN 0120            S1=0.0
ISN 0121            S2=0.0
ISN 0122            S3=0.0
ISN 0123            IF (NCBIN.EQ.1) GO TO 135
ISN 0125            DO 130 M=2,NCBIN
ISN 0126            S1=S1+CC(1,M)*(X1(K)-X2(K))**(M-1)
ISN 0127            S2=S2+CC(2,M)*(X1(K)-X3)**(M-1)
ISN 0128        130 S3=S3+CC(3,M)*(X2(K)-X3)**(M-1)
ISN 0129        135 S1=S1+CC(1,1)
ISN 0130            S2=S2+CC(2,1)
ISN 0131            S3=S3+CC(3,1)
ISN 0132            PC=X1(K)*P10+X2(K)*P20+X3*P30+X1(K)*X2(K)*S1+X1(K)*X3*S2+X2(K)*
                   1X3*S3+X1(K)*X2(K)*X3*(SOL(1)+SOL(2)*X1(K)+SOL(3)*X2(K))
ISN 0133            DEV=PC-P(K)
ISN 0134            DEVP=DEV/P(K)*100.D0
ISN 0135            WRITE(3,1140) X1(K),X2(K),P(K),PC,DEV,DEVP
ISN 0136            S=S+DEV*DEV
ISN 0137        140 SP=SP+DEVP*DEVP
ISN 0138            S=DSQRT(S/(NOMP-3))
ISN 0139            SP=DSQRT(SP/(NOMP-3))
ISN 0140        145 WRITE (3,1150) S,SP
ISN 0141            GO TO 10
ISN 0142        1000 FORMAT(10A8)
ISN 0143        1010 FORMAT (5I1,5X,4F10.5)
```

```
ISN 0144      1020 FORMAT(8F10.5)
ISN 0145      1030 FORMAT('1',//,3X,'PROGRAM 0040,BINARY AND TERNARY TOTAL PRESSURE
                  1FIT, J.POLAK, DEPT OF CHEM. ENG., U OF O.',/,3X,'PROGRAM NEW 26.5.
                  21972',/)
ISN 0146      1040 FORMAT (/,3X,'BINARY TOTAL PRESSURE',//,3X,   'P = P10*X1 + P20*X2
                  1 +X1*X2(C1 + C2(2X1-1) + C3(2X1-1)**2 + ...)',//,3X,10A8,//,3X,
                  2'T   =',F9.3,2X,'DEG.C.',/,3X,'P10 =',F9.3,3X,'P20 =',F9.3,/)
ISN 0147      1050 FORMAT (3X,'C',I1,' =',F12.5,'  (+-)',F12.5)
ISN 0148      1060 FORMAT(/,6X,'X1', 6X,'P EXP',3X,'P CALC',4X,'DEV',5X,'DEV %',/)
ISN 0149      1070 FORMAT(F10.4,2F9.2,F8.2,F9.2)
ISN 0150      1080 FORMAT (/,21X,'ST.DEV.',F8.2,F9.2,//)
ISN 0151      1090 FORMAT (/,3X,'TERNARY SYSTEM TOTAL PRESSURE',//,3X,   'P = P10*X1 +
                  1+ P20*X2 + P30*X3 + X1*X2(C11+C12(X1-X2)+...) + X1*X3(C21+C22(X1-X
                  23)+...) + X2*X3(C31+C32(X2-X3)+...)+',/,7X,'X1*X2*X3(C + D1*X1 + D
                  32*X2)')
ISN 0152      1095 FORMAT (/,3X,10A8,//,3X,'T   =',F9.3,'  DEG.C.',/,3X,'P10 =',F9.3,
                  23X,'P20 =',F9.3,3X,'P30 =',F9.3,/)
ISN 0153      1100 FORMAT (3X,'BINARY CONSTANTS:',/,3X,'(I,J)',6X,6('C(I,',I1,')',
                  17X),/)
ISN 0154      1110 FORMAT (3X,'(',I1,',J1,',6F13.5)
ISN 0155      1120 FORMAT(/,3X, 'TERNARY CONSTANTS:',3X,'C  =',F12.5,3X,'(+-)',F12.5,
                  1/,24X,'D1 =',F12.5,3X,'(+-)',F12.5,/,24X,'D2 =',F12.5,3X,'(+-)',
                  2F12.5)
ISN 0156      1130 FORMAT (/,6X,'X1',7X,'X2',7X,'P EXP',4X,'P CALC',5X,'DEV',5X,
                  1'DEV %',/)
ISN 0157      1140 FORMAT (1X,2F9.4,2F10.2,2F9.2)
ISN 0158      1150 FORMAT(/,32X,'ST.DEV.',2F9.2,//)
ISN 0159      1160 FORMAT (//,3X,'NO WOBBLING ON P-X CURVE OVER THE WHOLE CONCENTRATI
                  1ON RANGE')
ISN 0160      1170 FORMAT (3X,'MAXIMUM ON P-X CURVE FOR X =',F8.4,' AND P =',F9.2)
ISN 0161      1180 FORMAT (3X,'MINIMUM ON P-X CURVE FOR X =',F8.4,' AND P =',F9.2)
ISN 0162      1190 FORMAT (3X,'INFLEX  ON P-X CURVE FOR X =',F8.4,' AND P =',F9.2)
ISN 0163      1200 FORMAT ('+',40X,'LAST TWO CONSTS. ARE LIMITING VALUES OF P')
                                                                              MAIN
ISN 0164           END
```

```
      COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=45,SIZE=0000K,
                         SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,NOID,NOXREF
ISN 0002            REAL FUNCTION PCALC*8(X)
ISN 0003            IMPLICIT REAL*8(A-H,O-Z)
ISN 0004            COMMON X1(150),X2(150),P(150),CC(3,8),P10,P20,P30,NCOMP,NCBIN,N2
ISN 0005            COMMON ILIMIT
ISN 0006            IF (NCOMP.EQ.3) CALL EXIT
ISN 0008            XX2=1.D0-X
ISN 0009            S=0.0
ISN 0010            IF (ILIMIT.EQ.1) N2=N2-2
ISN 0012            IF (N2.EQ.1) GO TO 20
ISN 0014            DO 10 I=2,N2
ISN 0015         10 S=S+CC(1,I)*(2.D0*X-1.D0)**(I-1)
ISN 0016         20 S=S+CC(1,1)
ISN 0017            PCALC=X*P10+XX2*P20+X*XX2*S
ISN 0018            IF (ILIMIT.EQ.1) PCALC=X*CC(1,N2+1)+XX2*CC(1,N2+2)+X*XX2*S
ISN 0020            IF (ILIMIT.EQ.1) N2=N2+2
ISN 0022            RETURN                                                    PCALC
ISN 0023            END
```

```
      COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=45,SIZE=0000K,
                         SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,NOID,NOXREF

ISN 0002              REAL FUNCTION FEXP*8(X,I)
                    C   THIS FUNCTION MUST BE HERE, BECAUSE THAT  STUPID THING DOES NOT KNOW 0**0
ISN 0003              IMPLICIT REAL*8(A-H,O-Z)
ISN 0004              FEXP=1.D0
ISN 0005              IF (I.EQ.0) GO TO 20
ISN 0007              FEXP=X**I
ISN 0008           20 RETURN                                                        FEXP
ISN 0009              END
```

```
        COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=45,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,NOID,NOXREF
ISN 0002            REAL FUNCTION FREG*8(X,I)
ISN 0003            IMPLICIT REAL*8(A-H,O-Z)
ISN 0004            COMMON X1(150),X2(150),P(150),CC(3,8),P10,P20,P30,NCOMP,NCBIN,N2
ISN 0005            COMMON ILIMIT
ISN 0006            S=0.0
ISN 0007            IF (ILIMIT.EQ.1) N2=N2-2
ISN 0009            DO 10 K=1,N2
ISN 0010            V=2.D0*X-1.D0
ISN 0011            KM1=K-1
ISN 0012            KM2=K-2
ISN 0013         10 S=S+CC(1,K)*(-FEXP(V,K)+2.D0*KM1*(X-X*X)*FEXP(V,KM2))
ISN 0014            FREG=P10-P20+S
ISN 0015            IF (ILIMIT.EQ.1) FREG=CC(1,N2+1)-CC(1,N2+2)+S
ISN 0017            IF (ILIMIT.EQ.1) N2=N2+2
ISN 0019            RETURN                                                  FREG
ISN 0020            END
```

```
        COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=45,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,NOID,NOXREF
ISN 0002            REAL FUNCTION FSECD*8(X,I)
ISN 0003            IMPLICIT REAL*8(A-H,O-Z)
ISN 0004            COMMON X1(150),X2(150),P(150),CC(3,8),P10,P20,P30,NCOMP,NCBIN,N2
ISN 0005            COMMON ILIMIT
ISN 0006            S=0.0
ISN 0007            DO 10 K=1,N2
ISN 0008            V=2.D0*X-1.D0
ISN 0009            KM1=K-1
ISN 0010            KM2=K-2
ISN 0011            KM3=K-3
ISN 0012         10 S=S+CC(1,K)*(-2.D0*K*FEXP(V,KM1)+2.D0*KM1*(-FEXP(V,KM1)+2.D0*
                   1KM2*(X-X*X)*FEXP(V,KM3)))
ISN 0013            FSECD=S
ISN 0014            RETURN                                                  FSECD
ISN 0015            END
```

```
        COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=45,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,NOID,NOXREF
ISN 0002            REAL FUNCTION FCE*8(J,K)
ISN 0003            IMPLICIT REAL*8(A-H,O-Z)
ISN 0004            COMMON X1(150),X2(150),P(150),CC(3,8),P10,P20,P30,NCOMP,NCBIN,N2
ISN 0005            COMMON ILIMIT
ISN 0006            IF (NCOMP.EQ.3) GO TO 20
ISN 0008            IF (J.GT.N2) GO TO 10
ISN 0010            IF (J.EQ.(N2-1).AND.ILIMIT.EQ.1) GO TO 60
ISN 0012            IF (J.EQ.N2.AND.ILIMIT.EQ.1) GO TO 70
ISN 0014            V=2.D0*X1(K)-1.D0
ISN 0015            JM1=J-1
ISN 0016            FCE=X1(K)*(1.D0-X1(K))*FEXP(V,JM1)
ISN 0017            RETURN
ISN 0018         10 FCE=P(K)-X1(K)*P10-(1.D0-X1(K))*P20
ISN 0019            IF (ILIMIT.EQ.1) FCE=P(K)
ISN 0021            RETURN
ISN 0022         60 FCE=X1(K)
ISN 0023            RETURN
ISN 0024         70 FCE=1.D0-X1(K)
ISN 0025            RETURN
ISN 0026         20 X3=1.D0-X1(K)-X2(K)
ISN 0027            IF (J.GT.3) GO TO 30
ISN 0029            FCE=1.D0
ISN 0030            IF (J.EQ.2) FCE=X1(K)
ISN 0032            IF (J.EQ.3) FCE=X2(K)
ISN 0034            FCE=FCE*X1(K)*X2(K)*X3
ISN 0035            RETURN
ISN 0036         30 S1=0.0
ISN 0037            S2=0.0
ISN 0038            S3=0.0
ISN 0039            IF (NCBIN.EQ.1) GO TO 50
ISN 0041            DO 40 M=2,NCBIN
ISN 0042            S1=S1+CC(1,M)*(X1(K)-X2(K))**(M-1)
ISN 0043            S2=S2+CC(2,M)*(X1(K)-X3)**(M-1)
ISN 0044         40 S3=S3+CC(3,M)*(X2(K)-X3)**(M-1)
ISN 0045         50 S1=S1+CC(1,1)
ISN 0046            S2=S2+CC(2,1)
ISN 0047            S3=S3+CC(3,1)
ISN 0048            FCE=P(K)-X1(K)*P10-X2(K)*P20-X3*P30-X1(K)*X2(K)*S1-X1(K)*X3*S2-
                   2X2(K)*X3*S3
ISN 0049            RETURN                                                    FCE
ISN 0050            END
```

```
      COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=45,SIZE=0000K,
                         SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,NOID,NOXREF
                                                                          10
ISN 0002            SUBROUTINE REGULA(F,X1,X2,EPS, ITER)
                C   FALSE POSITION METHOD
ISN 0003            IMPLICIT REAL*8(A-H,O-Z)
ISN 0004            I=1
ISN 0005            A1=F(X1,ITER)
ISN 0006            A2=F(X2,ITER)
ISN 0007            IF (A1*A2) 90,70,70
ISN 0008         70 I=0
ISN 0009            GO TO 230
ISN 0010         90 DO 200 K=1,100
ISN 0011            X=(X2*A1-X1*A2)/(A1-A2)
ISN 0012            A=F(X,ITER)
ISN 0013            IF(A*A1) 130,170,170
ISN 0014        130 IF (DABS(X2-X).LE.EPS) GO TO 220
ISN 0016            X2=X
ISN 0017            A2=A
ISN 0018            GO TO 200
ISN 0019        170 IF (DABS(X1-X).LE.EPS) GO TO 220
ISN 0021            X1=X
ISN 0022            A1=A
ISN 0023        200 CONTINUE
ISN 0024        210 I=0
ISN 0025        220 X1=X
ISN 0026        230 ITER=I
ISN 0027            RETURN                                        REGULA
ISN 0028            END
```

```
        COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=45,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,NOID,NOXREF
ISN 0002            REAL FUNCTION FW*8(K,SOL)
ISN 0003            IMPLICIT REAL*8(A-H,O-Z)
ISN 0004            DIMENSION SOL(10)
ISN 0005            FW=1,D0
ISN 0006            RETURN
ISN 0007            END
```

FW

```
      COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=45,SIZE=0000K,
                         SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,NOID,NOXREF
ISN 0002                SUBROUTINE SQLIN (NOMC,NOMP,F,W,SOL,ERR,ICHECK,NOWF)                SQLIN 1
ISN 0003                IMPLICIT REAL*8(A-H,O-Z)                                            SQLIN 2
ISN 0004                DIMENSION AA(10,11),SOL(10),SOLPR(10),ERR(10)                       SQLIN 3
ISN 0005                NOMC1=NOMC+1                                                        SQLIN 4
ISN 0006                DO 19 M=1,20                                                        SQLIN 5
ISN 0007                IF (NOWF.EQ.1.AND.M.EQ.2) GO TO 20
ISN 0009                IF (M.EQ.1) GO TO 4                                                 SQLIN 7
ISN 0011                IF (M.EQ.2) GO TO 2                                                 SQLIN 8
ISN 0013                DO 1 N=1,NOMC                                                       SQLIN 9
ISN 0014                IF ((DABS((SOLPR(N)-SOL(N))/SOL(N))*100).GT.0.01D0) GO TO 2         SQLIN10
ISN 0016              1 CONTINUE                                                            SQLIN11
ISN 0017                GO TO 20                                                            SQLIN12
ISN 0018              2 DO 3 N=1,NOMC                                                       SQLIN13
ISN 0019              3 SOLPR(N)=SOL(N)                                                     SQLIN14
ISN 0020              4 DO 5 I=1,NOMC                                                       SQLIN15
ISN 0021                DO 5 J=1,NOMC1                                                      SQLIN16
ISN 0022              5 AA(I,J)=0.D0                                                        SQLIN17
ISN 0023                DO 8 I=1,NOMP                                                       SQLIN18
ISN 0024                IF (M.GT.1) GO TO 6                                                 SQLIN19
ISN 0026                WT=1.D0                                                             SQLIN20
ISN 0027                GO TO 7                                                             SQLIN21
ISN 0028              6 WT=W(I,SOL)                                                         SQLIN22
ISN 0029              7 DO 8 J=1,NOMC                                                       SQLIN23
ISN 0030                DO 8 K=J,NOMC1                                                      SQLIN24
ISN 0031                IF (J.EQ.K) AA(J,K)=AA(J,K)+F(J,I)**2*WT
ISN 0033                IF (J.EQ.K) GO TO 8
ISN 0035                AA(J,K)=AA(J,K)+F(J,I)*F(K,I)*WT
ISN 0036              8 CONTINUE                                                            SQLIN26
ISN 0037                DO 9 J=2,NOMC                                                       SQLIN27
ISN 0038                L=J-1                                                               SQLIN28
ISN 0039                DO 9 K=1,L                                                          SQLIN29
ISN 0040              9 AA(J,K)=AA(K,J)                                                     SQLIN30
ISN 0041                IF (ICHECK.NE.1) GO TO 11                                           SQLIN31
ISN 0043                WRITE(3,1000)                                                       SQLIN32
ISN 0044                DO 10 K=1,NOMC                                                      SQLIN33
ISN 0045             10 WRITE(3,1020) (AA(K,J),J=1,NOMC1)                                   SQLIN34
ISN 0046             11 CALL SOLVD (AA,10,NOMC,NOMC1,0.D0,DET,TEST)                         SQLIN35
ISN 0047                IF (ICHECK.NE.1) GO TO 13                                           SQLIN36
ISN 0049                WRITE(3,1030)                                                       SQLIN37
ISN 0050                DO 12 K=1,NOMC                                                      SQLIN38
ISN 0051             12 WRITE(3,1020) (AA(K,J),J=1,NOMC1)
```

```
ISN 0052          13 DO  14 K=1,NOMC                                          SQLIN39
ISN 0053          14 SOL(K)=AA(K,NOMC1)                                       SQLIN40
ISN 0054             S=0.D0                                                   SQLIN41
ISN 0055             DO 16 I=1,NOMP                                           SQLIN42
ISN 0056             S1=0.D0                                                  SQLIN43
ISN 0057             DO 15 J=1,NOMC                                           SQLIN44
ISN 0058          15 S1=S1+SOL(J)*F(J,I)                                      SQLIN45
ISN 0059             S1=S1-F(NOMC1,I)                                         SQLIN46
ISN 0060          16 S=S+S1*S1*W(I,SOL)                                       SQLIN47
ISN 0061             S=DSQRT(S/(NOMP-NOMC))                                   SQLIN48
ISN 0062             IF (ICHECK.NE.1) GO TO 17                                SQLIN49
ISN 0064             WRITE (3,1040) S                                         SQLIN50
ISN 0065          17 DO 18 K=1,NOMC                                           SQLIN51
ISN 0066          18 ERR(K)=S*DSQRT(AA(K,K))                                  SQLIN52
ISN 0067          19 CONTINUE                                                 SQLIN53
ISN 0068          20 RETURN                                                   SQLIN54
ISN 0069        1000 FORMAT(1X,//,3X,'NORMAL EQUATION MATRIX',/)              SQLIN55
ISN 0070        1020 FORMAT (3X,10(D13.5))                                    SQLIN56
ISN 0071        1030 FORMAT(1X,//,3X,'INVERSE MATRIX',/)                      SQLIN57
ISN 0072        1040 FORMAT (1X,//,3X,'SIGMA =',D13.5,///)                    SQLIN58
ISN 0073             END                                                      SQLIN**
```

```
        COMPILER OPTIONS - NAME=  MAIN,OPT=02,LINECNT=45,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,NOID,NOXREF
                                                                                SOLVD 1
ISN 0002              SUBROUTINE SOLVD (X,IX,M,N,PREC,DET,TEST)                 SOLVD 2
ISN 0003              INTEGER*2 I1(255), I2(255)                                SOLVD 3
ISN 0004              REAL*8 X(IX,N),T,DET,BIG,PREC,TEST,PIV,TEMP,DSQRT,DABS    SOLVD 4
ISN 0005              EQUIVALENCE (BIG,TEMP,PIV)                                SOLVD 5
ISN 0006              DET=1.0D0                                                 SOLVD 6
ISN 0007              TEMP=DABS(PREC)                                           SOLVD 7
ISN 0008              IF(TEMP.EQ.0.0D0) TEMP=0.5D-14                            SOLVD 8
ISN 0010              TEST=0.D0                                                 SOLVD 9
ISN 0011              DO 1 I=1,M                                                SOLVD10
ISN 0012              I2(I)=0                                                   SOLVD11
ISN 0013              DO 1 J=1,M                                                SOLVD12
ISN 0014            1 TEST=TEST+X(I,J)*X(I,J)                                   SOLVD13
ISN 0015              TEST=TEMP*DSQRT(TEST)/M                                   SOLVD14
ISN 0016              DO 9 K=1,M                                                SOLVD15
ISN 0017              BIG=0.D0                                                  SOLVD16
ISN 0018              DO 3 I=1,M                                                SOLVD17
ISN 0019              IF (I2(I).NE.0) GO TO 3                                   SOLVD18
ISN 0021              DO 2 J=1,M                                                SOLVD19
ISN 0022              IF (I2(J).NE.0) GO TO 2                                   SOLVD20
ISN 0024              T=DABS(X(I,J))                                            SOLVD21
ISN 0025              IF (T.LE.BIG) GO TO 2                                     SOLVD22
ISN 0027              BIG=T                                                     SOLVD23
ISN 0028              IROW=I                                                    SOLVD24
ISN 0029              JCOL=J                                                    SOLVD25
ISN 0030            2 CONTINUE                                                  SOLVD26
ISN 0031            3 CONTINUE                                                  SOLVD27
ISN 0032              IF (BIG.LE.TEST) RETURN                                   SOLVD28
ISN 0034              I1(K)=JCOL                                                SOLVD29
ISN 0035              I2(JCOL)=IROW                                             SOLVD30
ISN 0036              IF(JCOL.EQ.IROW) GO TO 6                                  SOLVD31
ISN 0038              DO 5 J=1,N                                                SOLVD32
ISN 0039              TEMP=X(IROW,J)                                            SOLVD33
ISN 0040              X(IROW,J)=X(JCOL,J)                                       SOLVD34
ISN 0041            5 X(JCOL,J)=TEMP                                            SOLVD35
ISN 0042              DET=-DET                                                  SOLVD36
ISN 0043            6 DET=DET*X(JCOL,JCOL)                                      SOLVD37
ISN 0044              PIV=1.D0/X(JCOL,JCOL)                                     SOLVD38
ISN 0045              DO 7 J=1,N                                                SOLVD39
ISN 0046              IF (J.NE.JCOL) X(JCOL,J)=PIV*X(JCOL,J)                    SOLVD40
ISN 0048            7 CONTINUE                                                  SOLVD41
ISN 0049              X(JCOL,JCOL)=PIV
```

```
ISN 0050          DO 9 I=1,M                                                SOLVD42
ISN 0051          IF (I.EQ.JCOL) GO TO 9                                    SOLVD43
ISN 0053          PIV=-X(I,JCOL)                                            SOLVD44
ISN 0054          DO 8 J=1,N                                                SOLVD45
ISN 0055          IF (J.NE.JCOL) X(I,J)=X(I,J)+PIV*X(JCOL,J)                SOLVD46
ISN 0057        8 CONTINUE                                                  SOLVD47
ISN 0058          X(I,JCOL)=PIV*X(JCOL,JCOL)                                SOLVD48
ISN 0059        9 CONTINUE                                                  SOLVD49
ISN 0060          DO 11 K=1,M                                               SOLVD50
ISN 0061          I=M+1-K                                                   SOLVD51
ISN 0062          JCOL=I1(I)                                                SOLVD52
ISN 0063          IROW=I2(JCOL)                                             SOLVD53
ISN 0064          IF(IROW.EQ.JCOL) GO TO 11                                 SOLVD54
ISN 0066          DO 10 I=1,M                                               SOLVD55
ISN 0067          TEMP=X(I,IROW)                                            SOLVD56
ISN 0068          X(I,IROW)=X(I,JCOL)                                       SOLVD57
ISN 0069       10 X(I,JCOL)=TEMP                                            SOLVD58
ISN 0070       11 CONTINUE                                                  SOLVD59
ISN 0071          TEST=0.D0                                                 SOLVD60
ISN 0072          RETURN                                                    SOLVD61
ISN 0073          END                                                       SOLVD**
```

APPENDIX V I

COMPUTER PROGRAM FOR THE EVALUATION OF THE REDLICH-KISTER CONSTANTS AND THE CALCULATION OF y, γ AND P calc BY THE INDIRECT METHOD

```
      DIMENSION Q(50),X(50),GI(50),GJ(50),TMI(50,5),TMJ(50,5),
     1   V(50,6),PM(5),Z(6,6)
      DIMENSION ZI(50),ZII(50),YY(50),PT(50),Y(50)
      DIMENSION TITLE(40)
      DO 6 I=1,5
    6 PM(I)=0.0
      READ(1,101)(PM(I),I=1,5)
      TL=0.00001
      FACT=1.0E0
    1 READ (1,1000)(TITLE(I),I=1,40)
 1000 FORMAT(40A2)
      WRITE(3,2000)(TITLE(I),I=1,40)
 2000 FORMAT (/1H1,40A2//)
      READ(1,100)N,NZ,MAX
      IF (N) 20,21,20
   20 READ(1,101)PCI,VCI,TCI,R,WI
      READ (1,101) PCII,VCII,TCII,R,WII
      READ (1,101)PI,PII,VLI,VLII,BJ,BII,TT
      K=1
  200 GO TO (201,202,203,208),K
  201 TR=TT/TCI
      U=WI
      GO TO 204
  202 TR=TT/TCII
      U=WII
      GO TO 204
  203 TCIII=(TCI*TCII)**.5
      WIII=(WI+WII)/2.0
      PCIII=4.00*TCIII*(PCI*VCI/TCI+PCII*VCII/TCII)/
     1   (VCI**(1./3.)+VCII**(1./3.))**3
      TR=TT/TCIII
      U=WIII
  204 BIII=(0.144500-0.3300/TR-0.1385/TR**2-0.0121/TR**3)+
     1   U*(0.073+0.4600/TR-0.50/TR**2-0.097/TR**3-0.007300/TR**8)
      GO TO (205,206,207,208),K
  205 BJ=R*TCI*BIII/PCI
      K=K+1
      GO TO 200
  206 BII=R*TCII*BIII/PCII
      K=K+1
      GO TO 200
  207 BIII=R*TCIII*BIII/PCIII
      K=K+1
```

```
0041            GO TO 200
0042        208 DIII=2.00*BIII-BJ-BII
0043            WRITE(3,102)BJ,BII,BIII,DIII
                C
0044            ZOI=(BJ-VLI)/R/TT
0045            ZOII=(BII-VLII)/R/TT
0046            DO 298 I=1,N
0047            READ(1,101)Q(I),X(I),Y(I)
0048            WRITE(3,102)Q(I),X(I),Y(I)
0049            XX=2.0*X(I)-1.0
0050            TMI(I,1)=1.0E0
0051            TMI(I,2)=4.0*X(I)-1.0
0052            TMI(I,3)=(6.0*X(I)-1.0)*XX
0053            TMI(I,4)=(8.0*X(I)-1.0)*XX**2
0054            TMI(I,5)=(10.0*X(I)-1.0)*XX**3
0055            TMJ(I,1)=1.0E0
0056            TMJ(I,2)=TMI(I,2)-2.0
0057            TMJ(I,3)=TMI(I,3)-4.0*XX
0058            TMJ(I,4)=TMI(I,4)-6.0*XX**2
0059            TMJ(I,5)=TMI(I,5)-8.0*XX**3
0060        298 CONTINUE
0061            WRITE(3,102)TL,(PM(I),I=1,5)
0062        297 NZ=NZ+1
0063            NZ1=NZ+1
0064            KK=0
0065        299 KK=KK+1
0066            M=0
0067        300 DO 410 I=1,N
0068            GI(I)=0.0
0069            GJ(I)=0.0
0070            DO 320 J=1,NZ
0071            GI(I)=GI(I)+PM(J)*TMI(I,J)
0072        320 GJ(I)=GJ(I)+PM(J)*TMJ(I,J)
0073            GI(I)=EXP((1.0-X(I))*(1.0-X(I))*GI(I))
0074            GJ(I)=EXP(X(I)*X(I)*GJ(I))
                C
0075            IF(KK-1)301,302,301
0076        302 ZI(I)=1.00
0077            ZII(I)=1.00
0078            GO TO 303
0079        301 ZI(I)=    (ZOI*(PT(I)-PI)
               1   +PT(I)*DIII*(1.00-YY(I))*(1.00-YY(I))/R/TT)
0080            ZII(I)=   (ZOII*(PT(I)-PII)
```

```
     1    +PT(I)*DIII*(YY(I)*YY(I))/R/TT)
0081       IF(ZI(I))304,305,306
0082   304 ZI(I)=1.00/EXP(-ZI(I))
0083       GO TO 307
0084   305 ZI(I)=1.00
0085       GO TO 307
0086   306 ZI(I)=EXP(ZI(I))
0087   307 IF(ZII(I))309,310,311
0088   309 ZII(I)=1.00/EXP(-ZII(I))
0089       GO TO 312
0090   310 ZII(I)=1.00
0091       GO TO 312
0092   311 ZII(I)=EXP(ZII(I))
0093   312 CONTINUE
0094       ZI(I)=1.00/ZI(I)
0095       ZII(I)=1.00/ZII(I)
0096   303 S=X(I)*PI*GI(I)*ZI(I)
0097       T=(1.0-X(I))*PII*GJ(I)*ZII(I)
0098       PT(I)=S+T
0099       YY(I)=S/PT(I)
0100       DO 400 J=1,NZ
0101       V(I,J)=S*(1.0-X(I))*(1.0-X(I))*TMI(I,J)
     1    +T*X(I)*X(I)*TMJ(I,J)
0102   400 CONTINUE
0103       V(I,NZ1)=(Q(I)-PT(I))*FACT
0104   410 CONTINUE
0105   500 DO 508 I=1,NZ1
0106       DO 508 J=1,NZ1
0107       SUM=0.0
0108       DO 509 K=1,N
0109   509 SUM=SUM+V(K,I)*V(K,J)
0110       Z(I,J)=SUM
0111       Z(J,I)=Z(I,J)
0112   508 CONTINUE
0113       DO 510 I=1,NZ
0114   510 WRITE(3,102)(Z(I,J),J=1,NZ1)
0115       CALL SOLVEJ(NZ,Z,INDIC)
         C
0116       DO 600 I=1,NZ
0117   600 PM(I)=PM(I)+Z(I,NZ1)
0118       WRITE(3,102)(Z(I,NZ1),I=1,NZ)
0119       M=M+1
0120       DO 612 I=1,NZ
```

```
0121            IF(ABS(Z(I,NZ1))-TL)612,612,616
0122          616 IF (M-11) 622,622,632
0123          622 GO TO 300
0124          612 CONTINUE
0125          632 WRITE (3,104)M,(PM(I),I=1,NZ)
                C
0126            DO 633 I=1,N
0127            V(I,NZ1)=V(I,NZ1)/FACT
0128          633 WRITE(3,102)Q(I),PT(I),V(I,NZ1),X(I),YY(I),GI(I),GJ(I),ZI(I),
                  1  ZII(I)
0129            IF(KK-3)299,700,700
                C     EVALUATION
0130          700 WRITE(3,105)
0131            WRITE(3,2000)(TITLE(I),I=1,40)
0132            WRITE(3,906)
0133          906 FORMAT(1H ,2X,4HPOBS,4X,5HPCOMP,3X,2HDP,6X,1HX,7X,1HY,7X,4HYOBS,4X
                  1,6HGAMMA1,2X,6HGAMMA2,2X,2HZI,6X,3HZII////)
0134            S=0.0
0135            T=0.0
0136            DO 750 I=1,N
0137            GI(I)=ALOG(GI(I))
0138            GJ(I)=ALOG(GJ(I))
0139            S=S+V(I,NZ1)*V(I,NZ1)
0140            T=T+ ABS(V(I,NZ1)/PT(I))
0141            WRITE(3,902)Q(I),PT(I),V(I,NZ1),X(I),YY(I),Y(I),GI(I),GJ(I),
                  1   ZI(I),ZII(I)
0142          902 FORMAT(1H ,3F8.2,2F8.3,3F8.4,2F7.3)
0143          750 CONTINUE
0144            WRITE(3,105)
0145            WRITE(3,922)(PM(I),I=1,NZ)
0146          922 FORMAT(1H ,2HB=,F10.5,3X,2HC=,F10.5,3X,2HD=,F10.5,3X,2HE=,F10.5,3X
                  1,2HF=,F10.5 )
0147            S=(S/(N-NZ))**0.5
0148            T=T/N*100.
0149            WRITE(3,907)N,NZ,TT,S,T
0150          907 FORMAT(21H NO.OF OBSERVATIONS =,I10/
                  1 18H NO.OF CONSTANTS =,I10/
                  2 22H SYSTEM TEMPERATURE AT,F10.2,5HDEG K/
                  3 26H ST.DEV. OF CORRELATION IS,F10.2,6HMM.HF./
                  4 27H AV.% DEV OF CORRELATION IS,F10.2/   )
0151            WRITE(3,2000)(TITLE(I),I=1,40)
0152            IF(NZ-MAX)297,760,760
0153          100 FORMAT (3I5)
```

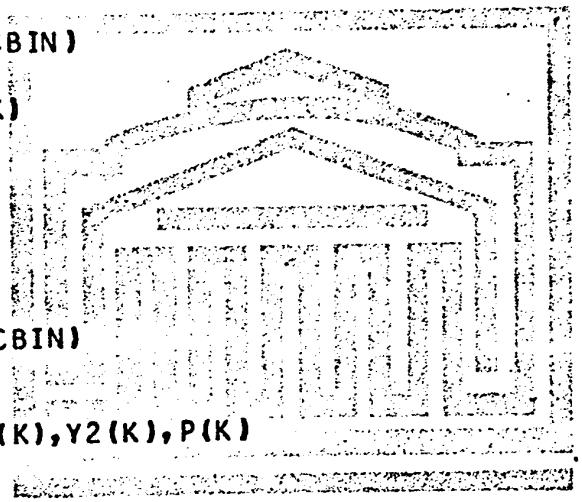
```
0154          101 FORMAT (8F10.0)
0155          102 FORMAT(1H ,9E14.6)
0156          104 FORMAT(//I5,5E15.7//)
0157          105 FORMAT(////)
0158          760 GO TO 1
0159           21 RETURN
0160              END
```

```
0001            SUBROUTINE SOLVFJ(NA,A,INDIC)
0002            DIMENSION A(6,6)
0003            NA1=NA+1
0004            DO 205 I=1,NA
0005            IF(A(I,I))200,206,200
0006        200 P=1./A(I,I)
0007            DO 201 J=I,NA1
0008        201 A(I,J)=P*A(I,J)
0009            DO 202 K=1,NA
0010            IF (I-K) 203,202,203
0011        203 Q=A(K,I)
0012            DO 204 J=I,NA1
0013        204 A(K,J)=A(K,J)-Q*A(I,J)
0014        202 CONTINUE
0015        205 CONTINUE
0016            INDIC=0
0017            RETURN
0018        206 IF(NZ-1) 300,304,300
0019        300 I1 = I+1
0020            DO 303 L=I1,NA
0021            IF(A(L,I)) 301,303,301
0022        301 DO 302 J=I,NA1
0023            HOLD=A(I,J)
0024            A(I,J)=A(L,J)
0025        302 A(L,J)=HOLD
0026            GO TO 200
0027        303 CONTINUE
0028            INDIC=1
0029        304 WRITE(3,207)I
0030        207 FORMAT(//25H DIAGONAL ELEMENT IN EQN ,I4,40H IS ZERO TRANSPOSE EQN
                1 WITH PREVIOUS ONE//)
0031            RETURN
0032            END
```

APPENDIX VII

COMPUTER PROGRAM FOR THE EVALUATION OF THE VAPOR COMPOSITION BY THE DIRECT METHOD

```
      C   PROGRAM 0041   CALCULATION OF BINARY AND TERNARY VAPOR COMPOSITION FROM
      C   TOTAL PRESSURE MEASUREMNET.,          DEPT.OF CHEM.ENG., U OF O.
      C   PROGRAM NEW 31.5.1972
0001        IMPLICIT REAL*8(A-H,O-Z)
0002        DIMENSION TITLE(10),        X1(50),X2(50),Y1(50),Y2(50),P(50)
0003        DIMENSION XMIMAX(10),YCALC(10)
0004        COMMON TEMP,V1,V2,B11,B22
0005        COMMON /CM1/ CC(3,8),P10,P20,P30,NCBIN,NCOMP
0006        EXTERNAL FMIMAX
0007        R=62361.8D0
0008     10 READ (1,1000) TITLE
0009        READ(1,1010) NCOMP,NCBIN,ICHECK,IPX,TEMP,P10,P20,P30
0010        IF (NCOMP.EQ.0) CALL EXIT
0011        READ(1,1020) B1,V1,B2,V2,B3,V3
0012        IF (NCOMP.EQ.3) GO TO 40
0013        READ(1,1020) (CC(1,I),I=1,NCBIN)
0014        DO 20 K=1,50
0015        READ(1,1020) X1(K),Y1(K),P(K)
0016        IF (IPX.EQ.1) P(K)=Y1(K)
0017        IF (X1(K).EQ.0.0) GO TO 30
0018     20 CONTINUE
0019     30 NOMP=K-1
0020        GO TO 80
0021     40 DO 50 K=1,3
0022     50 READ(1,1020) (CC(K,I),I=1,NCBIN)
0023        READ(1,1020) C,D1,D2
0024        DO 60 K=1,50
0025        READ(1,1020) X1(K),X2(K),Y1(K),Y2(K),P(K)
0026        IF (X1(K).EQ.0.0) GO TO 70
0027     60 CONTINUE
0028     70 NOMP=K-1
0029        CALL EXIT
0030     80 B11=B1
0031        B22=B2
0032        WRITE(3,1030) TITLE
0033        WRITE(3,1060) TEMP
0034        WRITE(3,1065) P10,B1,V1,P20,B2,V2
0035        DO 85 K=1,NCBIN
0036     85 WRITE(3,1070) K,CC(1,K)
0037        Z=0.0
0038        NMIMAX=0
0039        DO 110 K=1,99
0040        Z1=Z
```

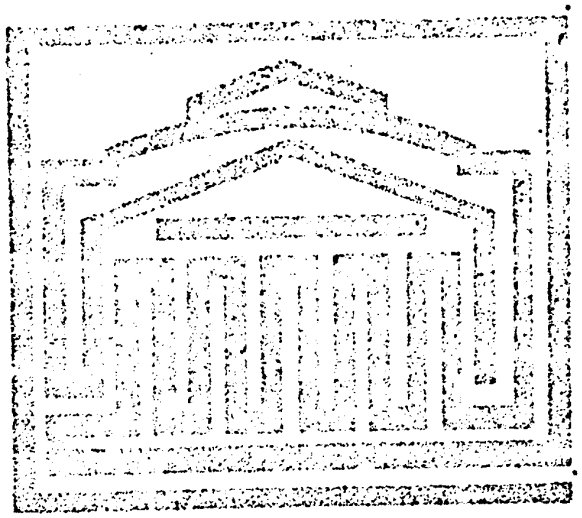


```
0041            Z2=Z1+0.01D0
0042            CALL REGULA (FMIMAX,Z1,Z2,0.0001D0,ITER)
0043            IF (ITER.EQ.0) GO TO 110
0044            NMIMAX=NMIMAX+1
0045            XMIMAX(NMIMAX)=Z1
0046        110 Z=Z2
0047            IF (NMIMAX.EQ.0) XMIMAX(1)=1.D0
0048            IF (NMIMAX.EQ.0) GO TO 140
0049            DO 120 K=1,NMIMAX
0050            TEST=PDP(3,XMIMAX(K),0.D0)
0051            IF (TEST.LT.0.0) WRITE(3,1080) XMIMAX(K)
0052            IF (TEST.GT.0.D0) WRITE(3,1090) XMIMAX(K)
0053        120 CONTINUE
0054            IF (NMIMAX.GT.1) WRITE(3,1100)
0055            NX0=0
0056            DO 130 K=1,NOMP
0057            IF (X1(K).GT.XMIMAX(1)) GO TO 150
0058        130 NX0=NX0+1
0059        150 WRITE(3,1110)
0060        140 WRITE(3,1035)
0061            H0=0.0005D0
0062            DP0=PDP(2,H0,0.D0)
0063            YH0=H0*(1.D0+DP0*PSI(H0))/(1.D0+H0*DP0*PSI(H0))
0064            S=0.0
0065            XI=H0
0066            YI=YH0
0067            IF (ICHECK.EQ.1) WRITE(3,1040) XI,YI
0068            DO 100 K=1,NOMP
0069            IF (X1(K).GT.XMIMAX(1)) GO TO 160
0070            H=(X1(K)-XI)/10.D0
0071            DO 90 L=1,10
0072            CALL RUNKU(XI,YI,H,YI1)
0073            XI=XI+H
0074            IF (ICHECK.EQ.1) WRITE(3,1040) XI,YI1
0075         90 YI=YI1
0076        100 YCALC(K)=YI1
0077            GO TO 175
0078        160 NDOWN=NOMP-NX0
0079            H0= 0.0005D0
0080            DP0=PDP(2,0.9995D0,0.D0)
0081            XI=0.9995D0
0082            YI=XI/(1.D0-PSI(XI)*DP0*H0)
0083            IF (ICHECK.EQ.1) WRITE(3,1040) XI,YI
```

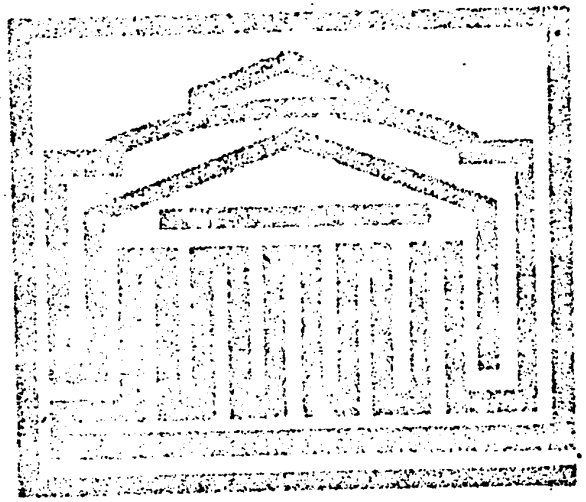
```
0084            DO 170 K=1,NDOWN
0085            I=NOMP-K+1
0086            H=(X1(I)-XI)/10.DO
0087            DO 180 L=1,10
0088            CALL RUNKU (XI,YI,H,YI1)
0089            XI=XI+H
0090            IF (ICHECK.EQ.1) WRITE(3,1040) XI,YI1
0091          180 YI=YI1
0092          170 YCALC(I)=YI1
0093          175 S=0.0
0094          200 DO 190 K=1,NOMP
0095              IF (IPX.EQ.1) Y1(K)=YCALC(K)
0096              DEV=YCALC(K)-Y1(K)
0097              S=S+DABS(DEV)
0098              WRITE(3,1040) X1(K),Y1(K),YCALC(K),DEV
0099              IF (K.GT.NXO) WRITE(3,1120)
0100          190 CONTINUE
0101              S=S/NOMP
0102              WRITE(3,1050) S
0103              GO TO 10
0104         1000 FORMAT (10A8)
0105         1010 FORMAT (I1,I1,I1,I1,6X,4F10.5)
0106         1020 FORMAT (8F10.5)
0107         1030 FORMAT('1',///,3X,'PROGRAM 0041  CALCULATION OF VAPOR PHASE COMPN.
                 1FROM TOTAL PRESSSURE MEASUREMENT',/,3X,'J.POLAK, DEPT.OF CHEM.ENG.
                 2, U OF O',/,3X, 'PROGRAM NEW 31.5.1972',///,3X,10A8)
0108         1035 FORMAT ( //,6X,'X1',5X,'Y1 EXP',3X,'Y1 CALC',3X,'DEV',/)
0109         1040 FORMAT (F10.4,3F9.4)
0110         1050 FORMAT (/,24X,'MEAN',F9.4)
0111         1060 FORMAT (//,3X,'T    =',F9.3,/,12X,'PO',8X,'BII',6X,'VI')
0112         1065 FORMAT (3X,'(1)',F11.3,F9.1,F10.3,/,3X,'(2)',F11.3,F9.1,F10.3,
                 1//,3X,'CONSTANTS FOR BINARY P-X FIT:')
0113         1070 FORMAT (3X,'C',I1,' =',F14.5)
0114         1080 FORMAT (/,3X,'MAXIMUM ON P-X FOR X=',F8.4)
0115         1090 FORMAT (/,3X,'MINIMUM ON P-X FOR X=',F8.4)
0116         1100 FORMAT (/,3X,'WARNING - MORE EXTREMES ON P-X CURVE')
0117         1110 FORMAT (/,3X,'FCR POINTS DESIGNATED BY *** INTEGRATION PROCEED FRO
                 1M X1=1',/)
0118         1120 FORMAT ('+',38X,'***')                                    MAIN
0119              END
```

```
0001          SUBROUTINE RUNKU (XI,YI,H,YI1)
0002          IMPLICIT REAL*8(A-H,O-Z)
0003          AK1=FRK(XI,YI)
0004          X=XI+0.5D0*H
0005          Y=YI+0.5D0*H*AK1
0006          AK2=FRK(X,Y)
0007          Y=YI+0.5D0*H*AK2
0008          AK3=FRK(X,Y)
0009          X=XI+H
0010          Y=YI+H*AK3
0011          AK4=FRK(X,Y)
0012          YI1=YI+H/6.D0*(AK1+2.D0*(AK2+AK3)+AK4)
0013          RETURN
0014          END
```

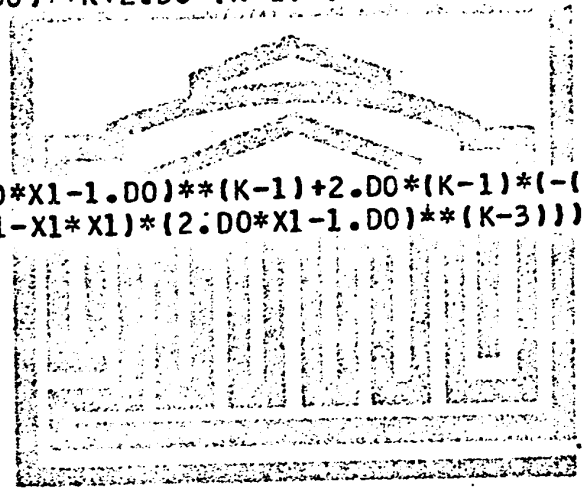
RUNKU



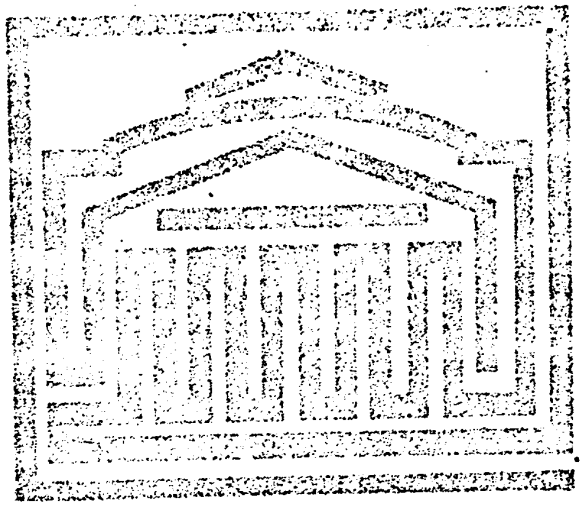
```
0001          REAL FUNCTION FRK*8(X,Y)
0002          IMPLICIT REAL*8(A-H,O-Z)
0003          COMMON T,V10,V20,B11,B22
0004          X2=1.DO-X
0005          RT=(T+273.15DO)*62361.8DO
0006          FRK=PSI(X)*Y*(1.DO-Y)/(Y-X)*PDP(2,X,0.DO)
0007          RETURN                                                    FRK
0008          END
```



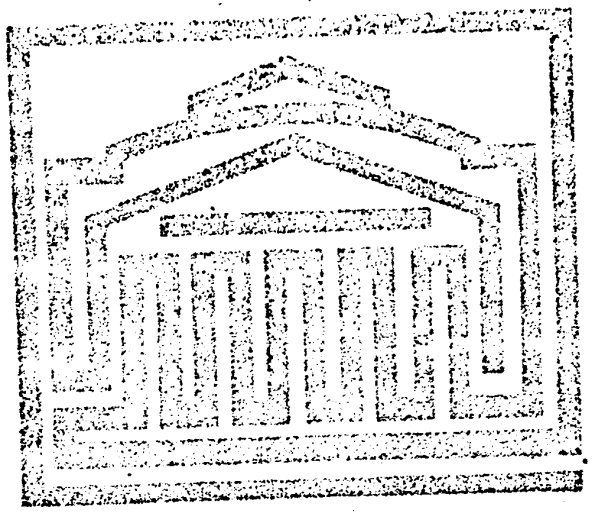
```
0001          REAL FUNCTION PDP*8(I,X1,X2)
0002          IMPLICIT REAL*8(A-H,O-Z)
0003          COMMON /CM1/ CC(3,8),P10,P20,P30,NCBIN,NCOMP
0004          IF (NCOMP.EQ.3) CALL EXIT
0005          XX2=1.D0-X1
0006          IF (I.EQ.2) GO TO 20
0007          IF (I.EQ.3) GO TO 40
0008          S1=0.0
0009          DO 10 K=1,NCBIN
0010       10 S1=S1+CC(1,K)*(X1-XX2)**(K-1)
0011          PDP=X1*P10+XX2*P20+X1*XX2*S1
0012          RETURN
0013       20 S1=0.0
0014          DO 30 K=1,NCBIN
0015       30 S1=S1+CC(1,K)*(-(2.D0*X1-1.D0)**K+2.D0*(K-1)*(X1-X1*X1)*(2.D0*X1-
             11.D0)**(K-2))
0016          PDP=P10-P20+S1
0017          RETURN
0018       40 S1=0.0
0019          DO 50 K=1,NCBIN
0020       50 S1=S1+CC(1,K)*(-2.D0*K*(2.D0*X1-1.D0)**(K-1)+2.D0*(K-1)*(-(2.D0*X1
             1-1.D0)**(K-1)+2.D0*(K-2)*(X1-X1*X1)*(2.D0*X1-1.D0)**(K-3)))
0021          PDP=S1
0022          RETURN
0023          END
```



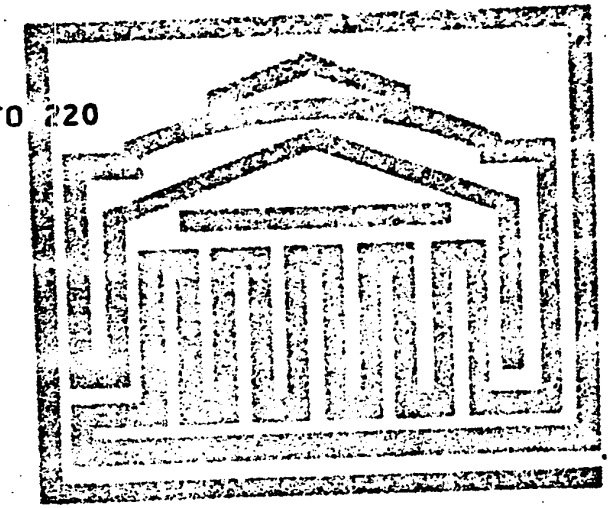
```
0001          REAL FUNCTION FMIMAX*8(X,I)
0002          IMPLICIT REAL*8(A-H,O-Z)
0003          FMIMAX=PDP(2,X,0.D0)
0004          RETURN                                                    FMIMAX
0005          END
```



```
0001          REAL FUNCTION PSI*8(X)
0002          IMPLICIT REAL*8(A-H,O-Z)
0003          COMMON TEMP,V1,V2,B1,B2
0004          PSI=(X*(B1-V1)+(1.DO-X)*(B2-V2))/62361.8DO/(TEMP+273.15DO)+1.DO
             1/PDP(1,X,0.DO)
0005          RETURN
0006          END
```

```
0001            SUBROUTINE REGULA(F,X1,X2,EPS, ITER)
                C   FALSE POSITION METHOD
0002                IMPLICIT REAL*8(A-H,O-Z)
0003                I=1
0004                A1=F(X1,ITER)
0005                A2=F(X2,ITER)
0006                IF (A1*A2) 90,70,70
0007            70  I=0
0008                GO TO 230
0009            90  DO 200 K=1,100
0010                X=(X2*A1-X1*A2)/(A1-A2)
0011                A=F(X,ITER)
0012                IF(A*A1) 130,170,170
0013            130 IF (DABS(X2-X).LE.EPS) GO TO 220
0014                X2=X
0015                A2=A
0016                GO TO 200
0017            170 IF (DABS(X1-X).LE.EPS) GO TO 220
0018                X1=X
0019                A1=A
0020            200 CONTINUE
0021            210 I=0
0022            220 X1=X
0023            230 ITER=I
0024                RETURN
0025                END
```



APPENDIX VIII

PHYSICAL PROPERTIES

	Benzene	n-Hexane	Cyclohexane
Pc (mm Hg)	36985	22510	30835
Vc (cc/g mole)	256.5	367.6	309.6
Tc (°K)	562.7	508.0	554.2
ω *	0.215	0.290	0.186
ρ_c	0.3045	0.2344	0.2718
ρ_{L_s}	0.30570	0.23387	0.27327
Mol. wt	78.108	86.172	84.156
a	6.90565	6.87773	6.84498
b	1211.033	1171.530	1203.526
c	220.79	224.366	222.863
d 25°C	0.87384	0.65490	0.77383

t°C	p** (mm Hg)			V^L*** (ml/g mole)		
	Benzene	n-Hexane	Cyclohexane	Benzene	n-Hexane	Cyclohexane
0	26.358	45.344	27.858	86.897	127.133	105.989
5	34.865	58.933	36.599	87.370	127.967	106.579
10	45.563	75.744	47.522	87.851	128.820	107.179
15	58.871	96.335	61.032	88.341	129.691	107.790
20	75.262	121.324	77.579	88.840	130.582	108.413
25	95.258	151.387	97.663	89.348	131.494	109.048

* NGPSA DATA BOOK 1966, NATURAL GAS PROCESSON SUPPLIER ASSOCIATION, TULSA, OKLAHOMA, P. 154-156, 74103

** $\log P = a - b/(t + c)$

*** $V^L = \text{Mol wt}/([1 + \alpha (1 - Tr) + \beta (1 - Tr)^{1/3}] \times \rho_{Ls})$

	Benzene	n-Hexane	Cyclohexane
$\alpha = 0.73098 + 0.28908\,\omega$	0.7931	0.8148	0.7847
$\beta = 1.75238 + 0.74293\,\omega$	1.9121	1.9678	1.8906

SECOND VIRIAL COEFFICIENTS

Pure Components

Temperature (°C)	n-Hexane	Cyclohexane	Benzene
0	-2451.8	-2165.8	-2046.3
5	-2316.5	-2043.8	-1923.2
10	-2194.1	-1934.0	-1813.0
15	-2082.8	-1834.7	-1713.8
20	-1981.2	-1744.5	-1624.2
25	-1888.1	-1662.3	-1542.9

Binary Mixtures

Temperature (°C)	Cyclohexane-Benzene	n-Hexane-Cyclohexane	n-Hexane Benzene
0	-2107.6	-2323.0	-2255.0
5	-1984.8	-2192.9	-2125.2
10	-1874.6	-2075.5	-2008.3
15	-1775.3	-1969.1	-1902.6
20	-1685.3	-1872.3	-1806.6
25	-1603.3	-1783.8	-1719.0