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AN INVESTIGATION OF ENHANCEMENT FACTOR MINIMIZATION  
WITH RECIPROCAL TEMPERATURE FOR BINARY MIXTURES  
CONTAINING HELIUM AND HYDROGEN

by

Diogenes A. Macias P.

Ingeniero Quimico

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A Thesis submitted to the Faculty and the Board of Trustees of the Colorado School of mines in partial fulfillment of the requirement for the degree of Master of Science. (C.P.R.)

Signed: Diogenes Macias P.  
Diogenes Macias P.

Golden, Colorado

Date June 9-1, 1978

Approved: ED Sloan  
E.D. Sloan  
Thesis Advisor

P.F. Dickson  
P.F. Dickson  
Head of Department

Golden, Colorado

Date June 9, 1978

To God

To my Sons

To my mother

To my Wife

To my Brothers

## ABSTRACT

This study investigated the behavior of the enhancement factor with respect to the reciprocal temperature for He-C<sub>2</sub>H<sub>6</sub>, He-Kr, H<sub>2</sub>-C<sub>6</sub>H<sub>6</sub> and H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> systems. A computer program was written to compute the enhancement factor with equations employing virial coefficients. The systems He-C<sub>2</sub>H<sub>6</sub>, He-Kr, H<sub>2</sub>-C<sub>6</sub>H<sub>6</sub> and H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> were tested in the temperature ranges 95.0°K - 230.0°K, 100.0°K - 150.0°K, 323.0°K - 523.0°K, and 83.0°K - 255.0°K, respectively. The pressure range was 0 to 150 atmospheres for all the binary systems mentioned.

The enhancement factor plotted against reciprocal temperature shows a minimum near the boiling point of the heavy component in the He-C<sub>2</sub>H<sub>6</sub>, He-Kr and H<sub>2</sub>-C<sub>6</sub>H<sub>6</sub> systems. The H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> was tested with twelve isotherms and no minimum was obtained, which is in agreement with the experimental work reported by Hiza, Heck and Kidnay [19].

The minimum in the enhancement factor versus reciprocal temperature plot was determined to be due to the enhancement factor equation term,  $2y_1 B_{11} \pi / RT$ . The solubility of gas in the liquid was determined to be a factor in this minimization. In systems where the solubility in the liquid phase is a factor, the mole fraction of the heavy component should be considered in the enhancement calculation.

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## INTRODUCTION

The study of systems composed of light and heavy binary mixtures has importance in extreme ranges of processing, such as cryogenics and high pressure aromatic hydrogenation.

The purpose of the work presented here is to investigate the existence of the minimum enhancement factor on an isobaric plot at reciprocal temperature of several light-heavy binary systems.

According to Hiza-Duncan [1], the minimum enhancement factor "may be unique" for the He-C<sub>2</sub>H<sub>6</sub> system. This work was done to determine the cause of the enhancement factor minimization for the He-C<sub>2</sub>H<sub>6</sub> and to determine if this minimization could be predicted for other systems.

A better understanding of the minimum in the enhancement factor in binary systems could produce an improvement in better prediction of separation of the heavy component from the light component.

## LITERATURE REVIEW

## I. Condition of Equilibrium

The condition of equilibrium for a solid-vapor and liquid vapor system may be written in terms of fugacity:

$$f_i^v = f_i^s = f_i^l \quad (1)$$

The variables are defined in the "Nomenclature" section.

For a component in a liquid solution the fugacity  $f_i^l$  can be expressed as:

$$f_i^l = X_i \gamma_i f_i^0 \quad (2)$$

The standard state  $f_i^0$  is a property of pure "i" when the activity coefficient  $\gamma_i$  reference state is 1.0 for the pure liquid.

The fugacity of component "i" in a binary system can be expressed in terms of volumetric behavior [16] as follows:

$$\ln \left( \frac{f_i}{\pi X_i} \right) = \frac{1}{RT} \int_V^\infty \left[ \left( \frac{\partial \pi}{\partial n_i} \right)_{T,V,n_j} - \frac{RT}{V} \right] dV - \ln Z \quad (3)$$

or as

$$\ln \left( \frac{f_i}{\pi X_i} \right) = \frac{1}{RT} \int_0^\pi \left[ \left( \frac{\partial V}{\partial n_i} \right)_{T,V,n_j} - \frac{RT}{\pi} \right] d\pi \quad (4)$$

Making the assumption of  $X_i = 1$ . and solving the equation (4), the fugacity of pure solid  $f_i^s$  can be written as

$$\ln \left( \frac{f_i^s}{\pi} \right) = \frac{1}{RT} \int_0^{P_1^0} \left[ \bar{V}_i^s - \frac{RT}{\pi} \right] d\pi + \frac{1}{RT} \int_{P_1^0}^\pi \left[ \bar{V}_i^s - \frac{RT}{\pi} \right] d\pi \quad (5)$$

If the effect of pressure on the volume of the solid is neglected, the equation (5) may be written as

$$f_i^s = p_i^o \phi_i^o \exp[\bar{v}_i^s (\pi - p_i^o)/RT] \quad (6)$$

Where the fugacity coefficient,  $\phi_i^o$ , of component "i" at its saturation pressure,  $p_i^o$  is

$$\ln \phi_i^o = \frac{1}{RT} \int_0^{p_i^o} \left[ v_i - \frac{RT}{\pi} \right] d\pi \quad (7)$$

The standard state fugacity of the liquid equals the liquid fugacity for the pure liquid and may be obtained from equation (6) as

$$f_i^o = p_i^o \phi_i^o \exp[\bar{v}_i (\pi - p_i^o)/RT] \quad (8)$$

Where the solubility in the liquid phase can not be neglected the equation for the fugacity of component "i" in the liquid becomes

$$f_i^L = \gamma_i x_i p_i^o \phi_i^o \exp[\bar{v}_i (\pi - p_i^o)/RT] \quad (9)$$

In equation (8) and (9) two corrections are applied. First the pure component fugacity coefficient  $\phi_i^o$  corrects for deviation of the saturated vapor from ideal gas behavior. Second, the exponential correction called "The Poynting correction", expresses the effect of pressure on the fugacity of solid phase.

Similarly the fugacity of the component "i" in the vapor phase is

$$f_i^v = \phi_i \pi Y_i \quad (10)$$

The  $\phi_i$  can be expressed by equation (3) or (4).

The enhancement factor,  $\epsilon$ , can be obtained by equating equations (6) and (10)

$$\epsilon = \frac{\pi Y_i}{p_i^o} = \left( \frac{\phi_i^o}{\phi_i} \right) \exp \left[ \bar{V}_i (\pi - p_i^o) / RT \right] \quad (11)$$

Combining equations (9) and (10) when the solubility of liquid phase can not be neglected and making  $\gamma_i = 1$ , the equation for the enhancement factor becomes:

$$\epsilon = \frac{\pi Y_i}{p_i^o} = X_i \left( \frac{\phi_i^o}{\phi_i} \right) \exp \left[ \bar{V}_i^s (\pi - p_i^o) / RT \right] \quad (12)$$

or

$$\ln(\epsilon) = \ln \left( \frac{\pi Y_i}{p_i^o} \right) = \ln X_i + \ln \phi_i^o + \bar{V}_i^s (\pi - p_i^o) / RT - \ln \phi_i \quad (13)$$

## II. Expanded Equation for the Enhancement Factor.

To integrate either equation (2) or (3) requires a good equation of state which has been proven satisfactory in predicting data for non ideal binary mixtures. The virial equation of state satisfies this condition and can be expressed as an equivalent pressures series:

$$PV/RT = 1 + B'\pi + C'\pi^2 + \dots \quad (14)$$

where  $B' = B/RT$  and

$$C' = (C - B^2)/(RT)^2$$

The virial equation of state has a sound theoretical background and demands no assumptions other than that the density is low enough for convergence. In extending the virial equation of state to mixtures the following mixing rules apply

$$B_{mix} = \sum_{i=1}^n \sum_{j=1}^n Y_i Y_j B_{ij} \quad (15)$$

$$C_{mix} = \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n Y_i Y_j Y_k C_{ijk} \quad (16)$$

Solving equation (4) and (5) using the virial equation of state, substituting for  $\phi_i^0$  and  $\phi_i$  in equation (7) and rearranging, the enhancement factor can be expressed as follows [16]:

$$\begin{aligned}
\ln(\epsilon) = & \bar{V}_1^s (\pi - p_1^s) / RT + B_{11} p_1^s / RT - (1 - Y_2^2) B_{11} \pi / RT + [C_{111} - B_{11}^2] p_1^s / 2(RT)^2 \\
& + (B_{22} - 2 B_{12}) Y_2^2 \pi / RT + [\pi^2 / 2(RT)^2] \left[ -3 Y_2^2 C_{122} - 6 Y_1 Y_2 C_{112} - 3 Y_1^2 C_{111} \right. \\
& + Y_2^3 (2 C_{222} - 4 B_{12} B_{22}) + Y_1 Y_2^2 (6 C_{122} + 4 B_{11} B_{22} + 8 B_{12}^2) \\
& + Y_1^2 Y_2 (12 B_{11} B_{12} + 6 C_{112}) + Y_1^3 (4 B_{11}^2 + 2 C_{111}) - Y_2^4 (3 B_{22}^2) \\
& - Y_1 Y_2^3 (12 B_{12} B_{22}) - Y_1^2 Y_2^2 (6 B_{11} B_{22} + 12 B_{12}^2) - Y_1^3 Y_2 (12 B_{11} B_{12}) \\
& \left. - Y_1^4 (3 B_{11}^2) \right] \quad , \quad (17)
\end{aligned}$$

Equation (17) is described as "the Expanded Equation" in this work. The concentration of the condensable (component 1) in the vapor phase, for the solid-vapor equilibria, is very small. Therefore, in a binary mixtures when  $y_1$  approaches zero,  $y_2$  approaches one and equation (17) can be reduced to the form: [16]

$$\begin{aligned}
 \ln(\epsilon) = & \bar{V}_1^* (\pi - \pi^0) / RT + B_{11} P_1^0 / RT + [ (C_{111} - 3B_{11}^2) (P_1^0)^2 ] / 2 (RT)^2 \\
 & + (B_{22} - 2B_{12}) \pi / RT + [ \pi^2 / 2 (RT)^2 ] [ -3C_{122} - 2C_{222} + 4B_{12}B_{22} \\
 & - 3B_{22}^2 ] \qquad \qquad \qquad (18)
 \end{aligned}$$

Equation (18) is described as "the Reduced Equation" in this work.

### III. Terms of Enhancement Factor Equation.

The terms in equation (17) for the enhancement factor were divided into three groups. The first term  $V_1^s (\pi - p_1^0) / RT$  defined as the "Poynting Correction" [16] and expresses the effect of pressure on the fugacity of the condensed phase.

The second group of terms is:

$B_{11} p_1^0 / RT + (C_{111} - B_{11}^2) (p_1^0)^2 / 2 (RT)^2$  which is classified as the logarithm of the fugacity coefficient for the pure component and is called "Phipure" in this work. The remaining terms in equation (17) were classified as the negative logarithm of the fugacity coefficient for component "1" in the mixture and is called "Phimixture" in this work.

#### A. Virial Coefficient Calculation Methods.

Virial coefficients of gases can be calculated from statistical mechanics, if the intermolecular potential between the molecules is known. The Lennard-Jones (6-12) intermolecular potential function is one model which has been widely used to describe the potential energy between nonpolar molecules. The major assumption is that the molecules are point centers whose force fields are spherically symmetric. This limits its application to very simple molecules. Even for simple molecules the representation is accurate only for restricted temperature ranges [21].

Kihara [11] has improved the Lennard-Jones potential by replacing the point center model with an impenetrable core whose dimensions are suggested by the geometry of the molecules. He retains the mathematical form of Lennard-Jones potential but the potential energy is now written, not a function of distance between molecular center, but rather as a function of the minimum distance between the cores.

Prausnitz and Myers [6] described a method for calculating the second cross virial coefficients using the Kihara potential equation for mixtures. This method was used for all

binary systems considered in this work.

A second method that was used in this work to calculate the virial coefficient was presented by Goodwin, Roder and Straty [4] which provides a very accurate fit to the second virial coefficient data for ethane [4]. The other method which was used from Goodwin, Roder and Straty [4] was for the calculation the third virial coefficient. Both methods are used for pure fluids only.

Little attention has been given to the third virial cross coefficient due to experimental difficulties, and the theoretical calculation using potential energy functions are tedious, for this reason good data or calculation for the third virial cross coefficient are scarce. However Chueh and Prausnitz [7] have presented a correlation of the third virial cross coefficients.

Hence there are four methods that have been used in obtaining the virial coefficients in this work:

- a) Kihara core model [11]
- b) Prausnitz and Myers [6]
- c) Chueh and Prausnitz method [7]
- d) Goodwin, Roder and Straty method [4]

These methods are discussed in detail in the following subsection.

a) Kihara core model.

Kihara retained the mathematical form of Lennard-Jones potential. The potential energy is given by the following relation [6]

$$U = U_0 \left[ \left( \frac{\rho_0}{\rho} \right)^{12} - 2 \left( \frac{\rho_0}{\rho} \right)^6 \right] \quad (19)$$

Using the potential energy given by equation and the methods of statistical mechanics Prausnitz and Myers [6] derived the second virial coefficient as

$$\frac{B}{N_0} = \frac{2}{3} \pi \rho_0^3 F_3 + M_0 \rho_0^2 F_2 + \left( S_0 + \frac{M_0^2}{4\pi} \right) \rho_0 F_1 + \left( V_0 + \frac{M_0 S_0}{4\pi} \right) \quad (20)$$

The parameters  $M_0$ ,  $S_0$ , and  $V_0$  may be calculated directly from the size and shape of the core. Most of the parameters  $M_0$ ,  $S_0$ , and  $V_0$  were taken from the predicted values of Prausnitz and Myers [6] ( see table B1 ) with one exception. For  $C_6H_6$  these parameters were not available in this literature and were obtained from the work by Brainard and Williams [22].

The three functions  $F_1$ ,  $F_2$  and  $F_3$  have the argument  $Z$  (where  $Z = U_0/kT$ ) and may be obtained from relations given by Kihara [11] :

$$F_s = \sum_{t=0}^{\infty} D_s^{(t)} Z^{\frac{6t-s}{12}} \quad (21)$$

For  $s = 1, 2, 3$

In order to obtain the values of  $F_i$  were used the coefficient  $\bar{D}_i^{(t)}$  (see table B2 ). In this thesis the calculation of second virial coefficient for He and H<sub>2</sub> were made without quantum corrections and satisfactory agreement of the data was obtained.

b) Prausnitz and Myers Method

The second virial cross coefficients were calculated by the method reported by Prausnitz and Myers [6]. Basically this method is the Kihara model used for gas mixture. The equation is:

$$\frac{B_{ij}}{N_0} = \frac{2}{3} \pi \rho_{ij}^3 F_3 + \frac{M_{oi} + M_{oj}}{2} \rho_{ij}^2 F_2 + \left( \frac{S_{oi} + S_{oj}}{2} + \frac{M_{oi} + M_{oj}}{4\pi} \right) \rho_{ij} F_1 + \frac{V_{oi} + V_{oj}}{2} + \frac{M_{oi} S_{oj} + M_{oj} S_{oi}}{8\pi} \quad (22)$$

Where  $F_1$ ,  $F_2$ , and  $F_3$  are functions that now depend on ( $U_{oij}/kT$ ) but are the same function as in equation (20). Of course equation (22) reduces to equation (20) when  $i=j$ . In order to calculate  $B_{ij}$  the core parameter for the pure component,  $U_{oij}$  and  $\rho_{oij}$  are required. The latter parameters, characterizing the potential function for interaction between unlike molecules, may be obtained from the semiempirical rule:

$$\rho_{oij} = 1/2(\rho_{oi} + \rho_{oj}) \quad (23)$$

$$U_{oij} = \sqrt{U_{oi} + U_{oj}} \quad (1 - k_{ij}) \quad (24)$$

Parameters for the equation (22) are given in Table B1 for all of the systems considered in this work.

c) Chueh and Prausnitz Method.

The third virial cross coefficient was calculated using the method of Chueh and Prausnitz [7] and this method is used for all binary systems considered in this work. The third virial coefficients are divided by  $V_c^2$  and are plotted against the reduced temperature  $T_r$ , using a procedure established by Chueh and Prausnitz [7]. The reduced third virial coefficients are given by generalized function:

$$\frac{C}{V_c^2} = f_c(T_r, d) \quad (25)$$

Where:

$$f_c = (0.232T_r^{-25} + .468T_r^{-5})(1 - e^{(1-1.89T_r^2)}) + d e^{-(2.48 - 2.3T_r + 2.7T_r^2)} \quad (26)$$

and  $T_r = T/T_c$

Equation (25) provides a useful correlation for reduced temperature between 0.8 and 1.75 and contains a parameter "d" which is some measure of the polarizability, size and shape of the molecule. The deviation function was determined by Chueh and Prausnitz [7] to be;

$$\frac{\Delta C}{V_c^2} = d e^{-(2.48 - 2.3T_r - 2.7T_r^2)} \quad (27)$$

The expression reported by Chueh and Prausnitz [7] to calculate the effective critical temperature is:

$$T_c = \frac{T_c^0}{1 + \frac{C_1^0}{mT}} \quad (28)$$

Where  $T_c^0$  is the classical critical temperature, that is, the effective critical temperature in the limit of high temperature. The effective critical volume is given by:

$$V_c = \frac{V_c^0}{1 + \frac{C_2^0}{mT}} \quad (29)$$

Where  $V_c^0$  is the classical critical volume.

The third virial coefficient of a mixture of N components is exactly related to the mole fraction  $Y_i, Y_j, Y_k, \dots$  by: [7]

$$C_{\text{mix}} = \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n Y_i Y_j Y_k C_{ijk} \quad (16)$$

For a binary system equation (16) becomes: [7]

$$C = Y_1^3 C_{111} + 3 Y_1^2 Y_2 C_{112} + 3 Y_1 Y_2^2 C_{122} + Y_2^3 C_{222} \quad (30)$$

Where  $C_{111}$  and  $C_{222}$  are the third virial coefficient for the component "1" and "2" and the cross coefficients  $C_{112}$  and  $C_{122}$  can be calculated from the equation:

$$C_{ijk} = (C_{ij} C_{ik} C_{jk})^{1/3} \quad (31)$$

Thus, the cross coefficient can be written as

$$C_{112} = (C_{11} C_{12} C_{12})^{1/3} \quad (32)$$

or 
$$C_{112} = (C_{11} C_{12}^2)^{1/3} \quad (33)$$

and 
$$C_{122} = (C_{12} C_{12} C_{22})^{1/3} \quad (34)$$

or 
$$C_{122} = (C_{22} C_{12}^2)^{1/3} \quad (35)$$

Where  $C_{11}$  is the same as  $C_{111}$  and  $C_{22}$  is the same as  $C_{222}$

The coefficient  $C_{12}$  is calculated from the equation

$$C_{ij} = V_{cij}^2 f_c (T/T_{cij}, d_{ij}) \quad (36)$$

and  $T_{cij}$  is calculated from [7]

$$T_{:ij} = \sqrt{T_{ci} \cdot T_{cj}} (1 - K_{ij}) \quad (37)$$

can be calculated from: [7]

$$V_{cij}^{1/3} = 1/2 (V_{:si}^{1/3} + V_{:ej}^{1/3}) \quad (38)$$

Equation (36) is the same as equation (25) but equation (36) is used for binary systems.

d) Method of Goodwin, Roder and Straty for pure virial coefficient of Ethane.

Goodwin, Roder, and Straty have formulated and demonstrated [4] an accurate empirical equation for determining the second virial coefficient of ethane using

$$B_{11} = 0.552671 - 1.106244/\chi - 0.592947/\chi^2 - 0.041944/\chi^{4.5} \quad (39)$$

Where  $\chi = T/T_c$

Third virial coefficients of ethane were calculated by the method of Goodwin, Roder, and Straty [4] as:

$$C_{111} = \left[ 0.244423/\chi + 0.832530/\chi^3 + 0.534880/\chi^5 \right] \left[ 1 - T_0/T \right] \quad (40)$$

$$\text{where } C_{111} = \left| 0.244423/\chi + 0.832530/\chi^3 + 0.534880/\chi^5 \right| \left| 1 - T_0/T \right|$$

$\chi = 1/T_c$

### B. Determination of Vapor Pressure.

In this work the vapor pressure of ethane was calculated from the equation described by Goodwin, Roder, and Straty [4]:

$$\ln(p^\circ) = -11.38996 + 18.84522\lambda - 7.63541\mu + 5.42844\mu^2 - 1.36232\mu^3 + 0.76924\mu(1-\mu)^{1.3} \quad (41)$$

$$\lambda = (1 - T_r/T) / (1 - T_r/T_c) \quad (42)$$

$$\mu = (T - T_r) / (T_c - T_r) \quad (43)$$

Goodwin, Roder, and Straty [4] have shown that this method of calculating of vapor pressure of ethane agrees well with experimental work (average deviation 1%).

The vapor pressure of benzene was not given in the vapor-liquid equilibrium data reported by Connolly [13]. There are several equations for the calculation of vapor pressure using the two parameter corresponding-states method. To achieve a greater accuracy, several investigators have proposed three parameter forms. The Pitzer [17] expansion is one of the more successful

$$\ln(\bar{P}_{\text{var}}) = \int \frac{f^{(0)}}{T} + \omega \int \frac{f^{(1)}}{T} \quad (44)$$

The functions  $\int \frac{f^{(0)}}{T}$  and  $\int \frac{f^{(1)}}{T}$  have been tabulated over wide ran-

ges of reduced temperature and have been expressed in analytical form by Lee and Kesler [17] as follows.

$$f^{(0)} = 5.927 - \frac{6.096}{T_r} - 1.288 \ln T_r + 0.169347 T_r^6 \quad (45)$$

and

$$f^{(1)} = 15.2518 - \frac{15.6875}{T_r} - 13.47 \ln T_r + 0.435 T_r^6 \quad (46)$$

The acentric factor for equation (53) was calculated by the equation of Lee and Kesler [17] and yields values of very close to those selected by Passut and Danner [23]

The equation for the acentric factor is:

$$\omega = \frac{-\ln P_c - 5.927 + 6.09648 \beta^{-1} + 1.2886 \ln \beta - 0.1693 \beta^6}{15.25 - 15.6875 \beta^{-1} - 13.4721 \ln \beta + 0.4357 \beta^6} \quad (47)$$

Where

$$\beta = T_b/T_c$$

The vapor pressure of Kr was taken from the values reported by Bowman [9].

### C. Determination of the Condensed Volume

The data for volume of benzene was also not available in the experimental work reported by Connolly. This volume can be calculated accurately by the Gunn and Yamada method [17].

This equation is:

$$\frac{V}{V_{sc}} = V_r^0 (1 - \omega \psi) \quad (48)$$

$V$  is the liquid specific volume,  $V_{sc}$  is a scaling parameter which is defined in terms of the volume at  $T_r=0.6$ .

If the volume at 0.6 is not available, then the values of  $V_{sc}$  can be estimated by

$$V_{sc} = \frac{R \bar{T}_c}{P_c} (0.292 - 0.0967\omega) \quad (49)$$

$\psi$  is calculated by

$$\psi = 0.29607 - 0.09045 T_r - 0.0484 T_r^2 \quad (50)$$

The values  $V_r^0$  is function of reduced temperature and can be calculated by:

$$V_r^0 = 0.33593 - 0.33953 T_r + 1.51941 T_r^2 - 2.02512 T_r^3 + 1.11422 T_r^4 \quad (51)$$

Substituting the values of  $\psi$ ,  $V_r^0$  and  $V_{sc}$  into the equation (48) yields the volume of benzene.

The data for the condensed volume of ethane were taken from Ziegler et al [3]. The data for condensed volume of Kr were taken from Cook [10].

## DATA SOURCES OF FOUR BINARY SYSTEMS

Table 1 reports the data source for the He-C<sub>2</sub>H<sub>6</sub>, He-Kr, H<sub>2</sub>-C<sub>6</sub>H<sub>6</sub>, and H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> systems.

TABLE 1. DATA SOURCES FOUR BINARY SYSTEM

System	Data source	Comments
He-C <sub>2</sub> H <sub>6</sub>	Miza and Duncan [1]	Six Isotherms: 150.0, 130.0, 122.0, 112.0, 102.0, and 95.0 °K.
	Heck [2]	Three Isotherms: 230.0, 200.0, and 170.0 °K.
	Ziegler, Kirk, Mullins and Berquist [3]	Volume of ethane
	Holborn and Otto [5]	Second and third virial coefficient of He for comparison with the Kihara potential k <sub>12</sub> = 0.4
	Miza and Duncan [30]	Seven Isotherms: 150.0, 140.0, 130.0, 120.0, 110.0, 105.0, and 100.0 °K. k <sub>12</sub> = 0.31
He-Kr	Kidnay, Miller and Miza [8]	Vapor pressure of Kr
	Miza and Duncan [30]	Volume of Kr
	Bowman [9]	Second and third virial coefficient for helium
	Cook [10]	
H <sub>2</sub> -C <sub>6</sub> H <sub>6</sub>	Holborn and Otto [5]	
	Connolly [13]	Five Isotherms: 523.0, 493.0, 0473.0, 453.0 and 433.0 °K
	Thompson and Edmlster [14]	Two Isotherms: 394.29 and 338.72 °K
	Coan and King [15]	One Isotherms: 323.16 °K k <sub>12</sub> = 0.4
H <sub>2</sub> -C <sub>2</sub> H <sub>6</sub>	Miza, Heck and Kidnay [19]	Nine Isotherms: 189.55, 169.40, 149.43, 130.0, 122.0, 108.0, 95.0, 87.0 and 81.0 °K
	Williams and Katz [20]	Three Isotherms: 255.38, 227.6, and 186.0 °K
	Ziegler, Kirk, Mullins and Berquist [3]	Volume of ethane
	Miza and Duncan [30]	k <sub>12</sub> = 0.055

#### METHODS AND EQUATIONS SOURCES OF FOUR BINARY SYSTEMS

The methods and equations used to obtain the different values of virial coefficients, vapor pressure and condensed volume have been described previously but they are tabulated in Table 2.

TABLE 2 METHODS AND EQUATIONS USED IN FOUR BINARY SYSTEMS

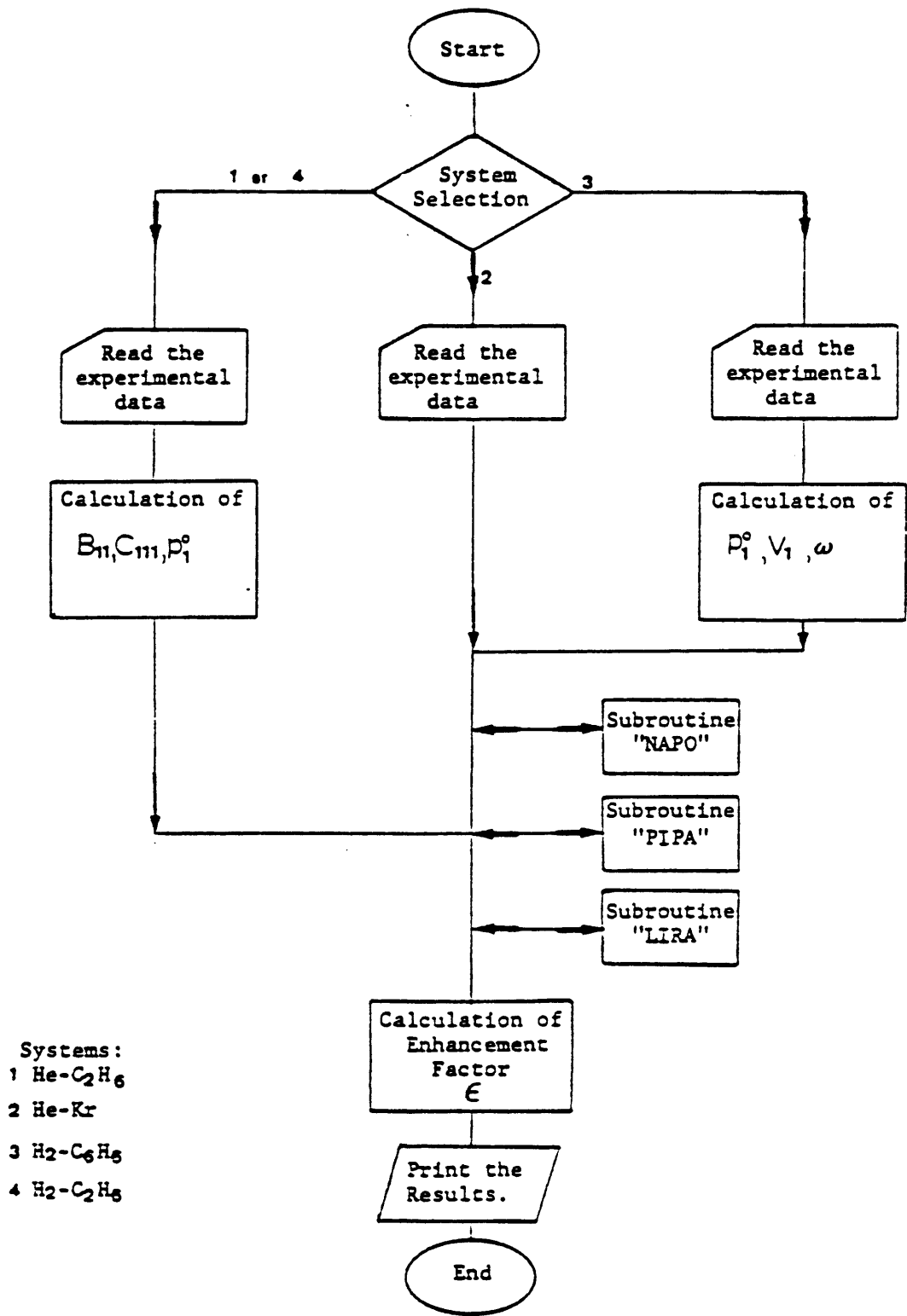
System	Methods & Equations	Comments
He-C <sub>2</sub> H <sub>6</sub>	Goodwin, Roder and Straty [6]	Equations for second and third virial coefficients of ethane. Equations for vapor pressure of ethane.
	Prausnitz and Myers [6] Kihara [11]	Second cross virial coefficients Second virial coefficients of He for comparison with values of Holborn and Otto [5]
	Chueh and Prausnitz [7]	Third cross virial coefficients
He-Kr	Prausnitz and Myers [6] Kihara [11] Sherwood-Prausnitz [12] Chueh-Prausnitz [7]	Second cross virial coefficients Second virial coefficients of Kr Third virial coefficients for Kr Third cross virial coefficients
H <sub>2</sub> -C <sub>6</sub> H <sub>6</sub>	Kihara [11]	Second virial for H <sub>2</sub> and C <sub>6</sub> H <sub>6</sub>
	Reid, Prausnitz and Sherwood [17]	Equation for acentric factor of benzene by Lee-Kesler
	Reid, Prausnitz and Sherwood [17]	Equation for vapor pressure of benzene by Pitzer
	Reid, Prausnitz and Sherwood [17]	Equation for volume of benzene by Gunn and Yamada
	Sherwood-Prausnitz [12] Prausnitz and Myers [6] Chueh and Prausnitz [7]	Third virial coefficients for benzene Second cross virial coefficients Third cross virial coefficients
H <sub>2</sub> -C <sub>2</sub> H <sub>6</sub>	Goodwin, Roder and Straty [6]	Equations for second and third virial coefficients for ethane and equation for vapor pressure of ethane
	Kihara [11] Prausnitz and Myers [6] Chueh and Prausnitz [7]	Second virial coefficients of H <sub>2</sub> Second cross virial coefficients Third cross virial coefficients

## COMPUTER PROGRAM

A computer program "Phase" was designed to compute the enhancement factor from equation (17) derived by Robinson-Hiza [16]. It is described in the flow chart in Figure 1 and the program listing with the subroutines is in appendix A. Basically, the computer program was applied for the He-C<sub>2</sub>H<sub>6</sub>, He-Kr, H<sub>2</sub>-C<sub>6</sub>H<sub>6</sub>, and H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> systems. The computer program differed slightly for each system because different experimental data were used; therefore it contains four parts: the main program and three subroutines.

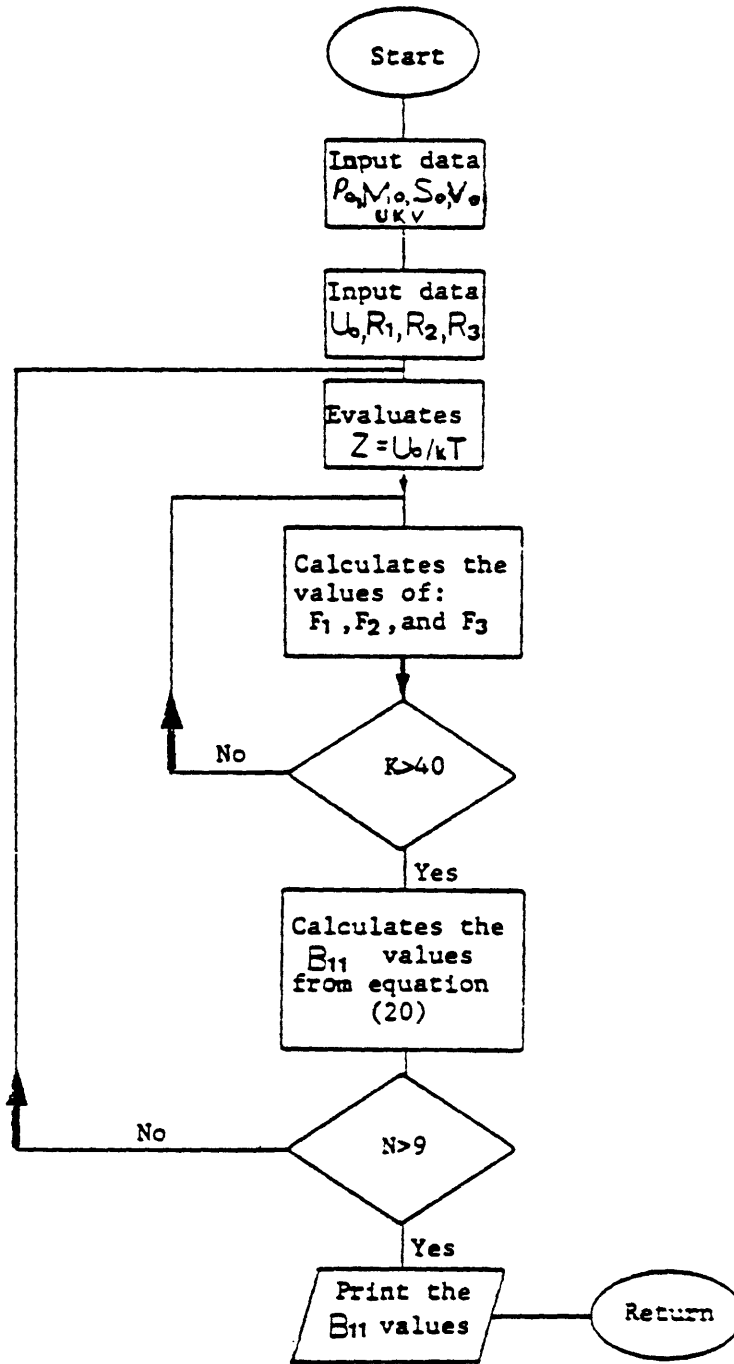
The virial coefficients are calculated in three subroutines. The first subroutine is called "Napo" and calculates the second virial coefficient for He, H<sub>2</sub>, Kr, and C<sub>6</sub>H<sub>6</sub>. This subroutine applied the equation derived by Kihara and used the function  $F_1$ ,  $F_2$ , and  $F_3$  of Kihara model [11]. The flow chart for this subroutine is in Figure 2. The second subroutine "Pipa" calculates the second cross virial coefficients for all the binary systems and used the method described by Prausnitz and Myers [6]. Essentially this method is the same as the Kihara, however, it includes pseudocritical parameters. The flow chart is shown in figure 3.

FIGURE No. 1



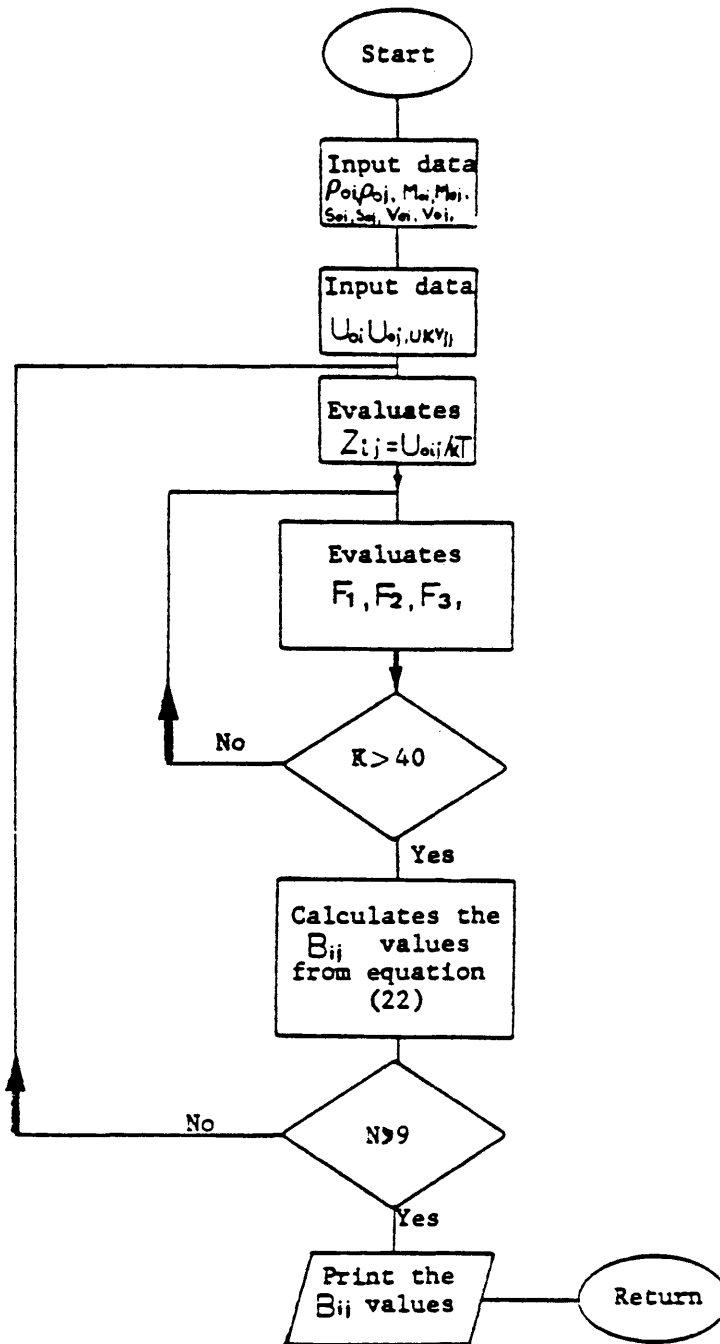
MAIN PROGRAM "PHASE"

FIGURE No. 2



SUBROUTINE "NAPO"

FIGURE No. 3



SUBROUTINE "PIPA"

The third subroutine " Lira " illustrated in Figure 4 calculates the third virial cross coefficients for all the systems mentioned before and was described by Chueh and Prausnitz [7]. In the main program the Goodwin, Roder and Straty [4] equations were used for He-C<sub>2</sub>H<sub>6</sub> and H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> systems in order to calculate the second and third virial coefficients and the vapor pressure of ethane. In the H<sub>2</sub>-C<sub>6</sub>H<sub>6</sub> system equation (57) of Gunn and Yamada [17] was used for the calculation of the volume of condensed component. Equation (56) of Lee and Kesler was used for calculation of acentric factor of benzene.

The third virial of C<sub>6</sub>H<sub>6</sub> and Kr were taken from the method of Sherwood and Prausnitz [12] using Kihara model and were input data in the computer program.

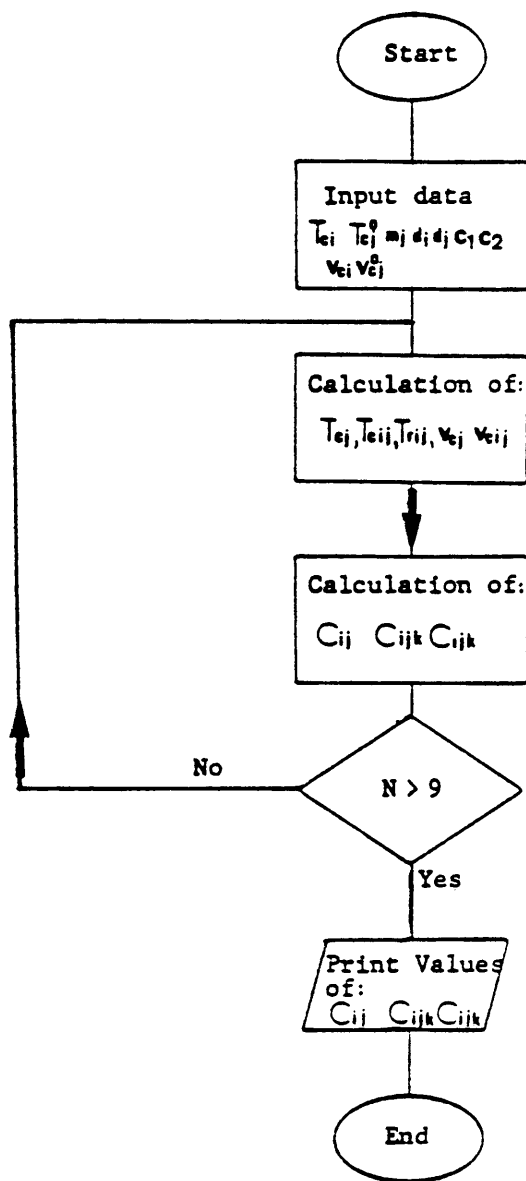
The third virial coefficients of He were taken from Holborn and Otto as reported by Dymond [5] and these values were also input data to the computer program in the main part.

The third virial coefficients of H<sub>2</sub> were also input data and were determined from Bird, Spotz and Hirschfelder [18].

The remaining input data in the main program consisted of

- 1) Total pressure
- 2) Temperature
- 3) Mole fraction of the heavy component
- 4) Critical constants.

FIGURE No. 4



SUBROUTINE "LIRA"

The first three of these were taken from the experimental work of each system, and last was taken from Smith and Van Ness [24].

## RESULTS AND DISCUSSION

The enhancement factors were calculated for the He-C<sub>2</sub>H<sub>6</sub>, He-Kr, H<sub>2</sub>-C<sub>6</sub>H<sub>6</sub> and H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> systems. These values are tabulated in table 3, 4, 5, and 6 respectively.

The predicted values for He-C<sub>2</sub>H<sub>6</sub> are given in the table 3. These values for the enhancement factor are in good agreement with those predicted by the experimental work. Hiza and Duncan [1] indicated that the values of the enhancement factor show an average deviation of 4% from the values predicted by Heck [2]. The values predicted in this work show a mean average deviation of 4.65% in the 230.0 °K, 200.0 °K, 170.0 °K and 150.0 °K isotherms as shown in Table 3.

The predicted values of the enhancement factor are in good agreement with those values of Hiza and Duncan [1]. The deviation in the results of the enhancement factor could be due to use the second virial cross and third virial cross coefficients which were obtained by theoretical rather than experimental means. The calculated values of the second virial coefficients by the method of Prausnitz and Myers [6] are in good agreement with the experimental data of other works [25, 26, 27, 28]; however such a comparison cannot be

TABLE 3. ENHANCEMENT FACTORS FOR THE He-C<sub>2</sub>H<sub>6</sub> SYSTEM

TEMP (°K)	VOL (cc/gmole)	P <sub>1</sub> <sup>0</sup> (atm)	Y <sub>1</sub>	π (atm)	ENHANCE. FACTOR EQN. (11)	ENHANCE. FACTOR EQN. (12)	EXPT. ENHANCE. FACTOR	PERDEV. BASED EQN.(12)	REF
=====									
k <sub>12</sub> = 0.4									
230.00	59.00	0.69E+01	0.45E+00	17.40	1.11	1.09	1.12	0.59	[2]
			0.30E+00	26.20	1.15	1.13	1.15	0.01	"
			0.20E+00	40.60	1.19	1.17	1.17	1.45	"
			0.14E+00	60.60	1.23	1.22	1.21	1.01	"
			0.10E+00	84.70	1.20	1.27	1.25	2.44	"
			0.74E-01	117.00	1.33		1.27	4.92	"
200.00	56.20	0.21E+01	0.25E+00	0.00	1.06	1.04	1.04	1.76	[2]
			0.92E-01	24.00	1.09	1.08	1.00	1.63	"
			0.49E-01	49.20	1.14	1.13	1.11	2.33	"
			0.31E-01	70.00	1.10	1.10	1.12	5.05	"
			0.24E-01	102.70	1.22	1.22	1.15	6.30	"
			0.10E-01	139.90	1.20	1.20	1.17	0.91	"
170.00	53.00	0.42E+00	0.29E-01	14.90	1.05	1.04	1.01	3.37	[2]
			0.15E-01	29.90	1.00	1.07	1.03	4.23	"
			0.90E-02	49.90	1.12	1.11	1.07	4.51	"
			0.66E-02	69.90	1.16	1.15	1.10	5.27	"
			0.53E-02	89.10	1.20	1.19	1.13	5.00	"
			0.41E-02	119.10	1.25	1.25	1.17	7.10	"

TABLE 3. ENHANCEMENT FACTORS FOR THE He-C<sub>2</sub>H<sub>6</sub> SYSTEM

TEMP (°K)	VOL (cc/gmole)	P <sub>1</sub> <sup>o</sup> (atm)	Y <sub>1</sub>	π (atm)	ENHANCE. FACTOR EQN. (11)	ENHANCE. FACTOR EQN. (12)	EXPT. ENHANCE. FACTOR	PERDEV. BASED EQN. (12)	REF
150.00	50.92	0.95E-01	0.37E-02	26.20	1.07	1.07	1.02	4.04	[1]
							1.06	5.79	"
							1.11	5.46	"
							1.10	9.19	"
							1.13	9.20	"
							1.17	8.96	"
130.00	49.15	0.13E-01	0.20E-02	4.50	1.02	1.02	1.02	0.47	"
							1.08	0.02	"
							1.15	-0.73	"
							1.23	0.70	"
							1.32	-3.03	"
							1.41	-4.20	"
122.00	40.46	0.46E-02	0.44E-03	10.72	1.04	1.04	1.04	0.25	"
							1.10	-4.33	"
							1.17	-3.24	"
							1.27	-3.23	"
							1.37	-4.02	"
							1.46	-6.01	"

TABLE 3. ENHANCEMENT FACTORS FOR THE He-C<sub>2</sub>H<sub>6</sub> SYSTEM

TEMP (°C)	VOL. (cc/gmole)	P <sub>i</sub> <sup>*</sup> (atm)	γ <sub>i</sub>	π (atm)	ENHANCE. FACTOR EQN. (11)	ENHANCE. FACTOR EQN. (12)	EXPT. ENHANCE. FACTOR	PERDEV. BASED EQN.(12)	REF
113.00	47.59	0.10E-02	0.10E-03	5.02	1.03	1.03	1.02	1.11	[1]
			0.00E-04	14.40	1.07	1.07	1.14	-6.03	"
			0.40E-04	25.72	1.12	1.12	1.22	-0.07	"
			0.29E-04	45.30	1.21	1.21	1.32	-0.13	"
			0.17E-04	99.60	1.46	1.46	1.64	-11.01	"
			0.15E-04	120.10	1.57	1.57	1.05	-15.19	"
102.00	46.47	0.17E-03	0.43E-04	3.90	1.02	1.02	1.06	-3.05	"
			0.15E-04	13.00	1.00	1.00	1.19	-9.46	"
			0.01E-05	26.00	1.15	1.15	1.31	-11.90	"
			0.54E-05	43.45	1.26	1.26	1.46	-14.11	"
			0.39E-05	60.00	1.40	1.40	1.55	-9.20	"
			0.27E-05	120.00	1.72	1.72	2.05	-16.19	"
95.00	46.20	0.36E-04	0.95E-05	4.10	1.03	1.03	1.12	-7.06	"
			0.42E-05	10.35	1.07	1.07	1.24	-13.76	"
			0.30E-05	15.32	1.11	1.11	1.32	-15.00	"
			0.20E-05	23.25	1.16	1.16	1.37	-14.00	"
			0.12E-05	46.20	1.33	1.33	1.56	-14.95	"
			0.11E-05	46.50	1.33	1.33	1.53	-13.09	"

done for the third virial coefficients due to the lack of availability of experimental data in the very low temperature regions.

The predicted values for the He-Kr system are tabulated in Table 4. These values are in good agreement (average deviation = 2.07%) with the experimental values reported by Kidnay, Miller and Hiza [8]. In this system the values of the enhancement factor were calculated using equation (13) which yielded little difference with the values calculated by Equation (11) as shown in Table 4. The deviation increases as the pressure increases.

The values of the enhancement factor for  $\text{H}_2\text{-C}_6\text{H}_6$  system are reported in Table 5. The values calculated from Equation (11) are in good agreement (average deviation = 3.9%) with the experimental work but the values calculated from Equation (13) are in better agreement (average deviation = 3.7%) with those reported experimentally.

The values predicted for  $\text{H}_2\text{-C}_2\text{H}_6$  are tabulated in Table 6. In general the data at 186.0 K, 227.6 K and 255.38 K were read from the graph [20] due to the inavailability of tabulated data; this led to a greater deviation from that predicted (average deviation = 3.67%). The predicted data for the other

TABLE 4. ENHANCEMENT FACTORS FOR THE He-Kr SYSTEM

TEMP (°K)	VOL (cc/gmole)	$P_1^0$ (atm)	$\gamma_1$	$\pi$ (atm)	ENHANCE. FACTOR EQN. (11)	ENHANCE. FACTOR EQN.(12)	EXPT. ENHANCE. FACTOR	PERDEV. REF BASED EQN.(12)
=====								
$k_{12} = 0.31$								
=====								
150.00	30.76	0.65E101	0.67E100	10.17	1.06	1.06	1.05	0.56
			0.36E100	20.10	1.13	1.13	1.12	0.00
			0.19E100	40.22	1.21	1.21	1.17	3.03
			0.10E100	80.20	1.35	1.34	1.20	5.00
			0.90E-01	100.00	1.43	1.41	1.30	0.10
			0.71E-01	120.00	1.46	1.43	1.33	7.06
=====								
140.00	37.21	0.30E101	0.42E100	9.09	1.00	1.07	1.07	0.42
			0.39E100	10.22	1.07	1.07	1.08	-0.54
			0.21E100	20.20	1.13	1.12	1.15	-2.19
			0.11E100	39.92	1.19	1.19	1.19	0.01
			0.59E-01	79.40	1.31	1.30	1.25	4.10
			0.44E-01	117.70	1.43	1.43	1.37	4.39
=====								
130.00	35.90	0.20E101	0.46E100	4.73	1.04	1.04	1.07	-2.67
			0.22E100	10.07	1.07	1.07	1.09	-1.65
			0.11E100	20.10	1.11	1.11	1.12	-0.90
			0.59E-01	41.60	1.19	1.18	1.21	-2.13
			0.34E-01	79.00	1.31	1.31	1.32	-1.10
			0.25E-01	119.00	1.44	1.43	1.46	-1.93

[0]

TABLE 4. ENHANCEMENT FACTORS FOR THE He-Kr SYSTEM

TEMP (°C)	VOL (cc/gmole)	$P_1^0$ (atm)	$\gamma_1$	$\pi$ (atm)	ENHANCE. FACTOR EQN. (11)	ENHANCE. FACTOR EQN. (12)	EXPT. ENHANCE. FACTOR	PERDEV. REF BASED EQN.(12)
120.05	34.04	0.11E101	0.12E100	9.00	1.06	1.06	1.05	1.12
			0.59E-01	20.00	1.10	1.10	1.10	0.09
			0.32E-01	39.09	1.10	1.17	1.10	0.51
			0.10E-01	79.50	1.32	1.32	1.34	-1.76
			0.10E-01	01.20	1.33	1.32	1.31	0.76
			0.13E-01	120.00	1.46	1.45	1.47	-1.15
								[ 8 ]
117.09	34.50	0.00E100	0.31E100	2.62	1.03	1.03	1.02	0.59
			0.45E-01	20.00	1.10	1.10	1.12	-1.72
			0.25E-01	39.05	1.10	1.10	1.24	-4.00
			0.13E-01	79.40	1.33	1.32	1.32	0.31
			0.13E-01	00.60	1.33	1.33	1.32	0.63
			0.90E-02	115.50	1.46	1.45	1.40	3.61
115.00	29.75	0.67E100	0.16E100	4.20	1.03	1.03	1.03	0.24
			0.36E-01	20.20	1.09	1.09	1.09	0.01
			0.19E-01	40.20	1.16	1.16	1.16	0.24
			0.12E-01	64.60	1.33	1.23	1.16	6.16
			0.11E-01	00.40	1.20	1.20	1.20	0.32
			0.02E-02	106.60	1.36	1.36	1.30	4.44

TABLE 4. ENHANCEMENT FACTORS FOR THE He-Kr SYSTEM

TEMP (°C)	VOL. (cc/gmole)	$P_1^*$ (atm)	$\gamma_1$	$\pi$ (atm)	ENHANCE. FACTOR EQN. (11)	ENHANCE. FACTOR EQN. (12)	EXPT. ENHANCE. FACTOR	PERDEV REF BASED EQN.(12)
110.00	29.31	0.39E100	0.10E100	4.02	1.03	1.03	1.02	0.74
			0.42E-01	10.09	1.05	1.05	1.07	-1.70
			0.21E-01	20.04	1.09	1.09	1.08	0.69
			0.11E-01	39.90	1.16	1.16	1.15	0.02
			0.65E-02	00.00	1.30	1.30	1.32	-1.56
0.53E-02	105.00	1.30	1.30	1.30	1.42	-2.04		
105.00	29.10	0.22E100	0.55E-01	4.10	1.03	1.03	1.03	0.44
			0.23E-01	10.00	1.05	1.05	1.06	-0.96
			0.12E-01	19.02	1.09	1.09	1.07	1.70
			0.65E-02	39.30	1.17	1.17	1.15	1.50
			0.45E-02	59.00	1.25	1.25	1.22	2.24
0.36E-02	00.00	1.32	1.32	1.31	1.31	1.07		
100.00	20.90	0.12E100	0.12E-01	10.00	1.05	1.05	1.04	1.04
			0.36E-02	19.60	1.09	1.09	1.00	0.70
			0.25E-02	37.60	1.17	1.17	1.16	0.90
			0.24E-02	59.90	1.20	1.20	1.23	3.60
			0.19E-02	79.30	1.36	1.36	1.30	4.50
0.10E-02	00.70	1.36	1.36	1.26	1.26	0.25		

[0]  
0

TABLE 5. ENHANCEMENT FACTORS FOR THE  $H_2-C_6H_6$  SYSTEM

TEMP (°K)	VOL (cc/gmole)	$P_1^0$ (atm)	$Y_1$	$\pi$ (atm)	ENHANCEMENT FACTOR EQN. (11)	ENHANCEMENT FACTOR EQN. (12)	EXPT. ENHANCEMENT FACTOR	PERDEV. REF BASED EQN. (12)
=====								
$k_{12} = 0.4$								
523.16	141.17	0.29E102	0.90E100	35.35	1.08	1.08	1.08	0.34 [13]
			0.00E100	43.23	1.17	1.17	1.17	0.05 "
			0.61E100	85.53	1.77	1.77	1.76	0.16 "
			0.39E100	140.10	2.32	2.01	1.83	9.83 "
=====								
473.16	129.90	0.19E102	0.61E100	38.21	1.23	1.21	1.20	0.51 "
			0.51E100	48.72	1.33	1.29	1.28	0.79 "
			0.39E100	70.02	1.40	1.41	1.39	1.28 "
			0.26E100	119.20	1.64	1.64	1.62	1.60 "
=====								
473.16	123.60	0.14E102	0.51E100	33.51	1.22	1.19	1.20	-0.20 "
			0.39E100	46.04	1.30	1.27	1.27	-0.04 "
			0.26E100	75.00	1.46	1.39	1.40	-0.71 "
			0.26E100	134.20	2.37	2.15	2.40	-13.36 "

TABLE 5. ENHANCEMENT FACTORS FOR THE H<sub>2</sub>-C<sub>6</sub>H<sub>6</sub> SYSTEM

TEMP (°K)	VOL (cc/gmole)	P <sub>1</sub> <sup>0</sup> (atm)	Y <sub>1</sub>	π (atm)	ENHANCE. FACTOR EQN. (11)	ENHANCE. FACTOR EQN. (12)	EXPT. ENHANCE. FACTOR	PERDEV. REF BASED EQN.(12)
453.16	110.12	0.10E102	0.51E100	22.03	1.15	1.14	1.14	0.23
					1.20	1.17	1.19	-1.56
					1.42	1.35	1.30	-2.32
					1.72	1.55	1.64	-5.59
453.16	113.34	0.70E101	0.39E100	20.67	1.14	1.13	1.13	0.40
					1.19	1.17	1.19	-1.58
					1.39	1.32	1.40	-5.19
					1.40	1.30	1.48	-6.74
394.27	105.63	0.30E101	0.25E100	13.67	1.09	1.00	1.11	-2.30
					1.15	1.13	1.16	-2.55
					1.24	1.17	1.25	-6.01
					1.30	1.31	1.44	-9.34

[13]

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TABLE 5. ENHANCEMENT FACTORS FOR THE H<sub>2</sub>-C<sub>6</sub>H<sub>6</sub> SYSTEM

TEMP (°K)	VOL (cc/gmole)	$p_i^0$ (atm)	$\gamma_i$	$\pi$ (atm)	ENHANCE. FACTOR EQN. (11)	ENHANCE. FACTOR EQN. (12)	EXPT. ENHANCE. FACTOR	PERDEV BASED EQN.(12)	REF
339.72	97.10	0.62E+00	0.50E-01	13.22	1.06	1.05	1.06	-0.80	[13]
			0.20E-01	34.25	1.11	1.10	1.12	-1.41	"
			0.11E-01	69.80	1.21	1.17	1.24	-5.07	"
			0.05E-02	116.12	1.34	1.29	1.50	-10.37	"
323.16	95.17	0.36E+00	0.17E-01	22.40	1.07	1.07	1.06	1.04	[15]
			0.10E-01	39.00	1.12	1.11	1.15	-3.21	"
			0.06E-03	59.70	1.19	1.18	1.23	-9.84	"
			0.71E-03	73.60					"

TABLE 6. ENHANCEMENT FACTORS FOR THE  $H_2-C_2H_6$  SYSTEM

TEMP (°K)	VOL (cc/gmole)	$P_1^0$ (atm)	$\gamma_1$	$\pi$ (atm)	ENHANCE. FACTOR EQN. (12)	ENHANCE. FACTOR EQN.(11)	EXPT. ENHANCE. FACTOR	PERDEV REF BASED EQN.(12)
=====								
$k_{12} = 0.05500$								
255.30	65.60	0.15E+02	0.52E+00	34.01	1.22	1.25	1.20	1.15
			0.42E+00	47.62	1.35	1.40	1.34	0.82
			0.35E+00	61.22	1.47	1.55	1.44	2.04
			0.32E+00	68.03	1.51	1.61	1.50	0.77
			0.24E+00	102.44	1.79	1.97	1.79	0.19
			0.22E+00	136.05	2.20	2.52	2.10	4.63
=====								
227.60	60.90	0.64E+01	0.48E+00	15.22	1.12	1.13	1.15	-2.79
			0.24E+00	34.01	1.20	1.30	1.20	-0.53
			0.19E+00	47.62	1.40	1.44	1.45	-3.45
			0.17E+00	61.22	1.53	1.60	1.64	-6.47
			0.12E+00	102.44	1.90	2.05	1.94	-1.73
			0.10E+00	136.05	2.25	2.50	2.23	0.06
=====								
109.47	55.70	0.13E+01	0.67E-01	24.90	1.27	1.25	1.29	-4.04
			0.46E-01	40.90	1.39	1.42	1.45	-4.43
			0.36E-01	60.10	1.50	1.64	1.66	-4.56
			0.29E-01	90.70	1.95	2.05	2.03	-4.02
			0.27E-01	120.20	2.36	2.53	2.47	-4.41
			0.26E-01	143.50	2.73	2.96	2.87	-4.92
=====								

TABLE 6. ENHANCEMENT FACTORS FOR THE H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> SYSTEM

TEMP (°K)	VOL (cc/gmole)	P <sub>1</sub> <sup>o</sup> (atm)	Y <sub>1</sub>	π (atm)	ENHANCE. FACTOR EQN. (12)	ENHANCE. FACTOR EQN. (11)	EXPT. ENHANCE. FACTOR	PERDEV. BASED EQN.(12)	REF
106.00	55.25	0.111E+01	0.70F-01	17.01	1.15	1.17	1.10	4.30	[20]
			0.43E-01	34.01	1.32	1.35	1.36	2.46	"
			0.33F-01	47.62	1.46	1.50	1.46	0.29	"
			0.25E-01	61.22	1.59	1.64	1.52	4.03	"
			0.20E-01	102.44	2.11	2.22	1.90	10.98	"
			0.10E-01	136.05	2.65	2.77	2.27	16.63	"
169.40	53.17	0.41E+00	0.15E-01	40.20	1.46	1.49	1.53	-4.45	[19]
			0.12E-01	60.70	1.74	1.79	1.84	-5.55	"
			0.11E-01	88.70	2.70	2.29	2.40	0.29	"
			0.10E-01	120.00	2.01	2.97	3.10	-9.52	"
			0.11E-01	154.30	3.37	3.59	3.82	-11.77	"
			0.11E-01	147.90	3.44	3.68	3.86	-10.80	"
149.62	50.97	0.92E-01	0.50E-02	21.70	1.31	1.32	1.36	-3.46	[19]
			0.39E-02	30.00	1.61	1.63	1.65	-2.60	"
			0.33E-02	60.00	2.04	2.09	2.10	-6.27	"
			0.31E-02	80.00	2.76	2.85	2.96	-6.90	"
			0.30E-02	118.90	3.75	3.91	3.99	-6.11	"

TABLE 6. ENHANCEMENT FACTORS FOR THE H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> SYSTEM

TEMP (°K)	VOL. (cc/gmole)	P <sub>i</sub> <sup>o</sup> (atm)	Y <sub>i</sub>	π (atm)	ENHANCE. FACTOR EQN. (12)	ENHANCE. FACTOR EQN. (11)	EXPT. ENHANCE. FACTOR	PERDEV. BASED EQN. (12)	REF
130.00	49.15	0.13E-01	0.14E-02	10.00	1.19	1.20	1.16	2.93	[19]
									"
									"
									"
									"
122.00	40.50	0.56E-02	0.55E-03	10.37	1.24	1.24	1.27	-2.79	[19]
									"
									"
									"
									"
100.00	47.24	0.52E-03	0.65E-04	25.60	2.04	2.06	3.23	-2.26	[19]
									"
									"
									"
									"

TABLE 6. ENHANCEMENT FACTORS FOR THE  $H_2-C_2H_6$  SYSTEM

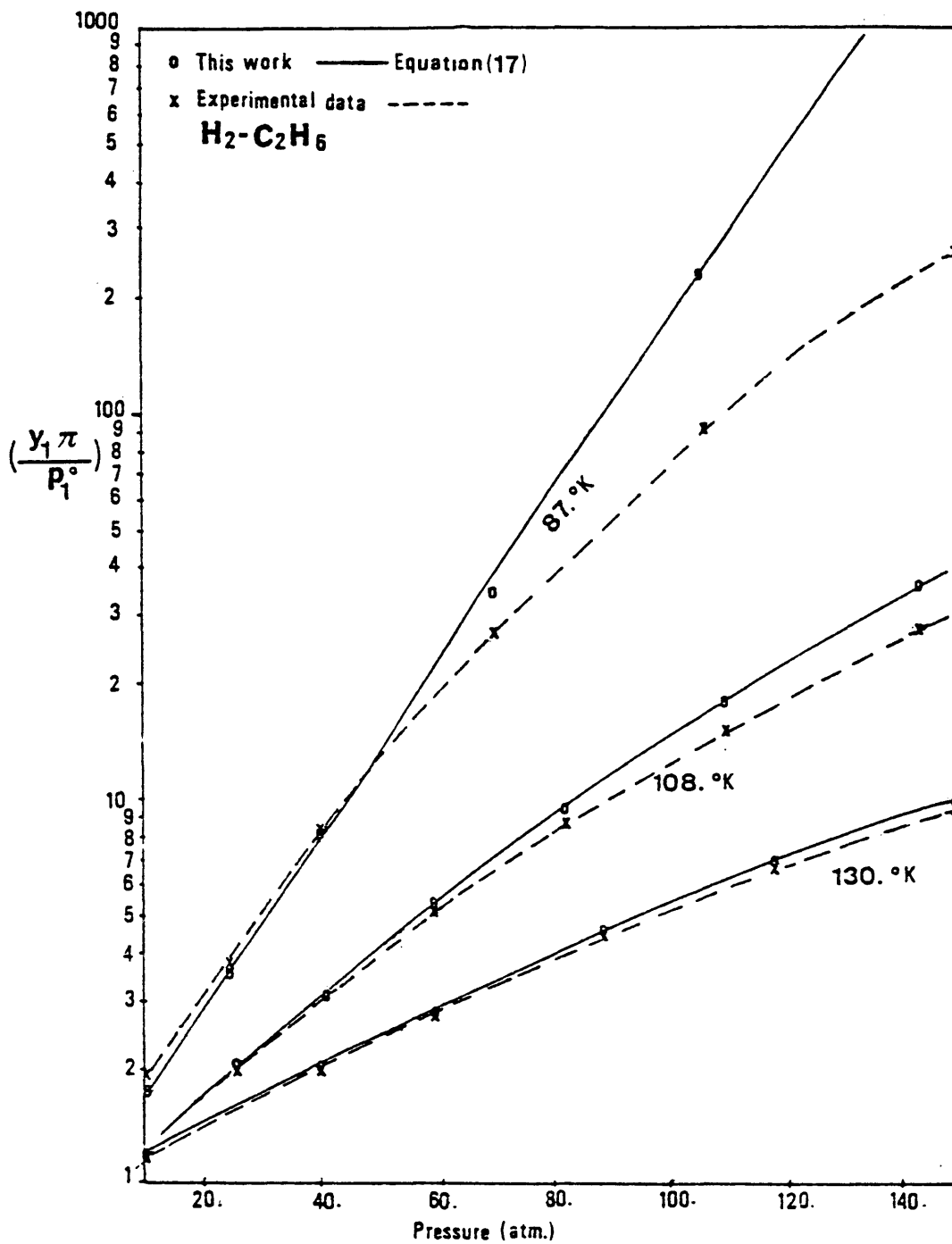
TEMP (°K)	VOL, (cc/gmole)	$P_1^0$ (atm)	$\gamma_1$	$\pi$ (atm)	ENHANCE. FACTOR EQN. (12)	ENHANCE. FACTOR EQN. (11)	EXPT. ENHANCE. FACTOR	PERDEV. BASED EQN (12)	REF
95.00	46.20	0.36E-04	0.57E-05	9.90	1.40	1.48	1.62	8.34	[19]
				24.62	2.65	2.65	2.92	9.16	"
				39.30	4.70	4.70	4.92	4.40	"
				69.40	14.66	14.66	13.00	6.26	"
				109.20	60.35	60.35	42.50	42.00	"
87.00	45.60	0.44E-05	0.69E-06	10.71	1.77	1.77	1.93	10.07	[19]
				25.60	3.66	3.66	3.00	5.69	"
				41.26	8.08	8.08	7.99	1.17	"
				70.60	35.61	35.61	27.00	20.00	"
									"
83.00	45.26	0.13E-05	0.21E-06	7.30	1.52	1.52	1.64	7.05	[19]
				24.01	4.23	4.23	4.57	7.52	"
				40.50	10.64	10.64	10.00	6.45	"
				71.00	65.90	65.90	40.70	61.91	"
									"

isotherms are in good agreement (average deviation = 4.7%) with those published by Hiza, Heck and Kidnay [19]. Experimental values of enhancement factor of the  $H_2-C_2H_6$  are plotted against pressure and are compared with the calculated values of this work in Figure 5 for three low temperature isotherms. In the same way experimental values of the enhancement factor are plotted against reciprocal temperature and compared with the predicted values of this work at pressures 140.0, 80.0, and 30.0 atmospheres in Figure 6.

The temperature dependence of the enhancement factor for the  $He-C_2H_6$  system predicted by the expanded equation (17) and the reduced Equation (18) are compared in the Figures 7, 8, and 9 at 30.0, 60.0, and 100.0 atmospheres respectively. For the  $He-C_2H_6$  system the expanded Equation (17) clearly shows a minimum enhancement factor near the normal boiling point of ethane (184.52°K), while the reduced Equation (18) predicts no minimum. This indicates that the minimum is a function of  $Y_1$ .

The values of the enhancement factor plotted against reciprocal temperature for He-Kr system, using the Equation (17) and (18), are plotted in the Figures 10 and 11 at 60.0 and 100.0 atmospheres. Equation (17) shows a minimum value for the enhancement factor near the normal boiling point of Kr

FIGURE No. 5



Enhancement Factor Versus Pressure of H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> System

FIGURE No. 6

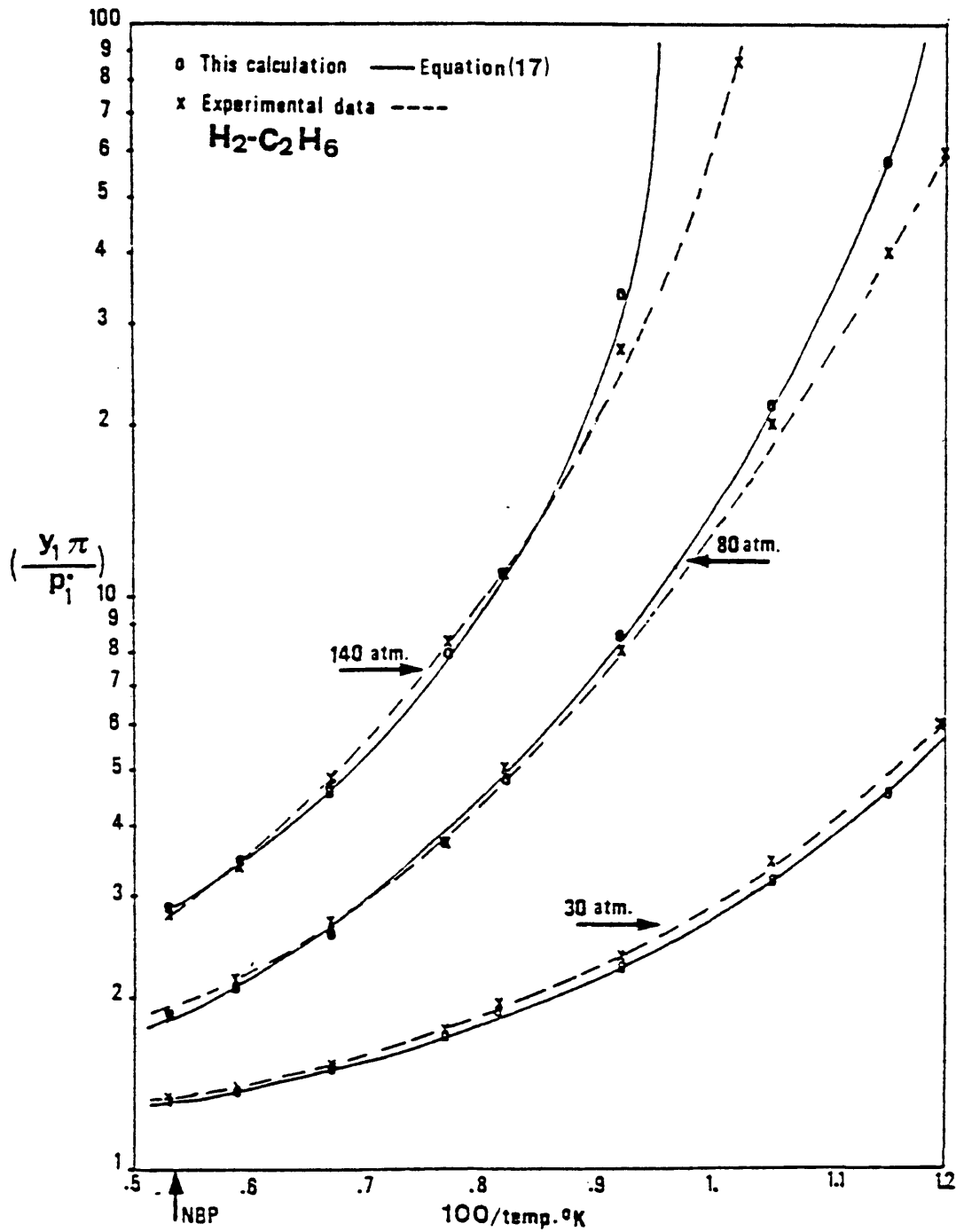
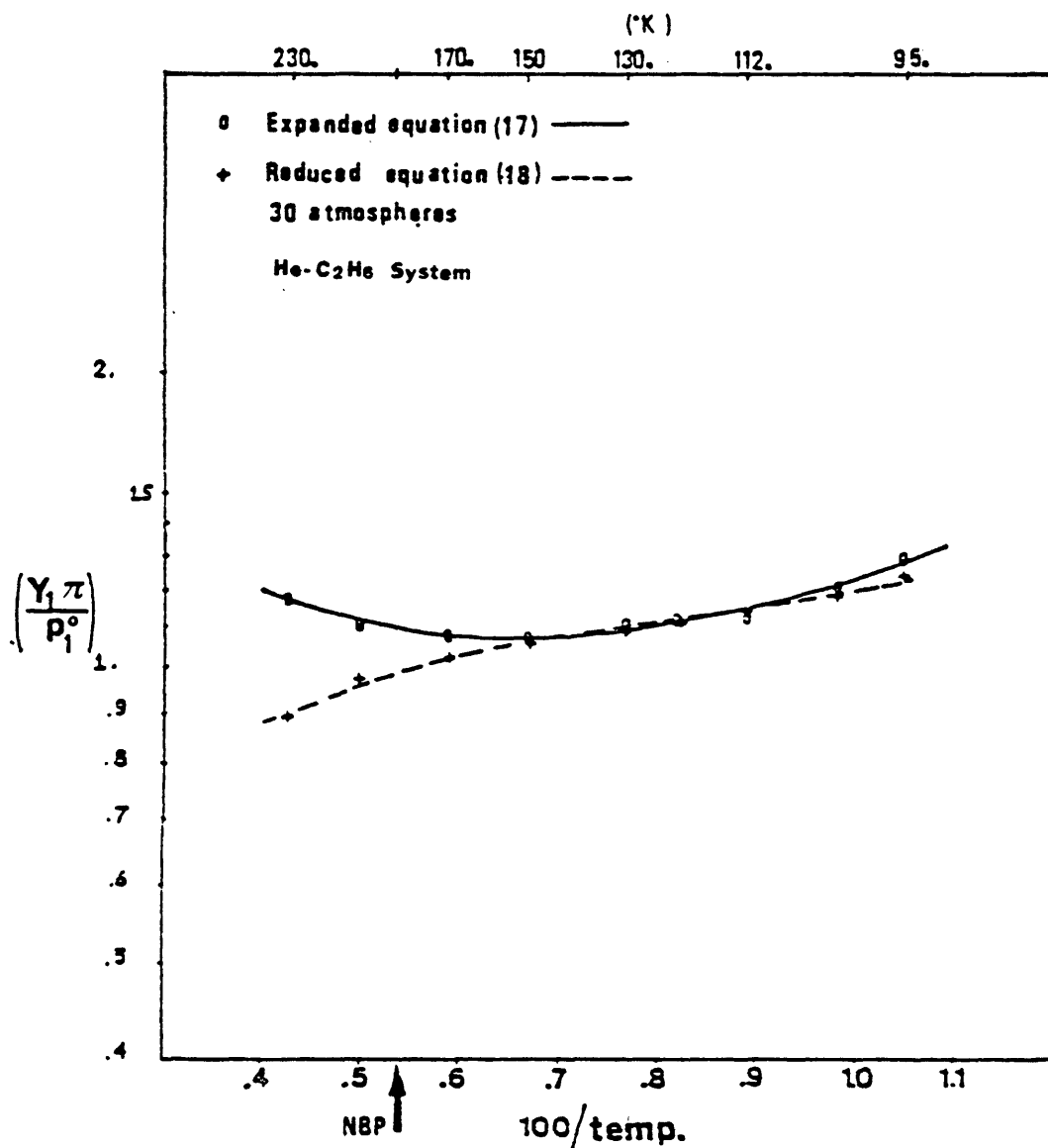
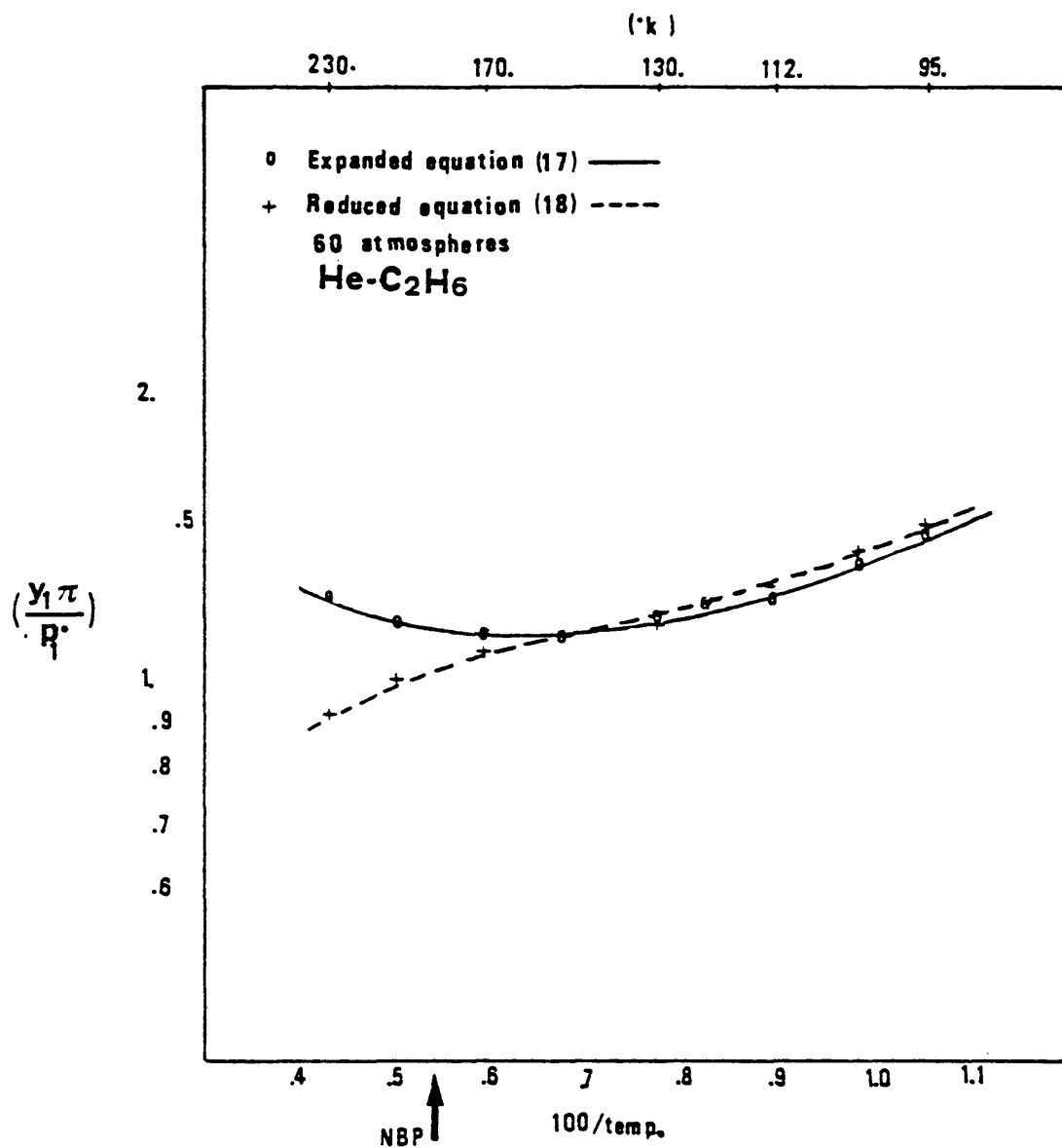
Enhancement Factor Versus Reciprocal Temperature of H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> System

FIGURE No. 7



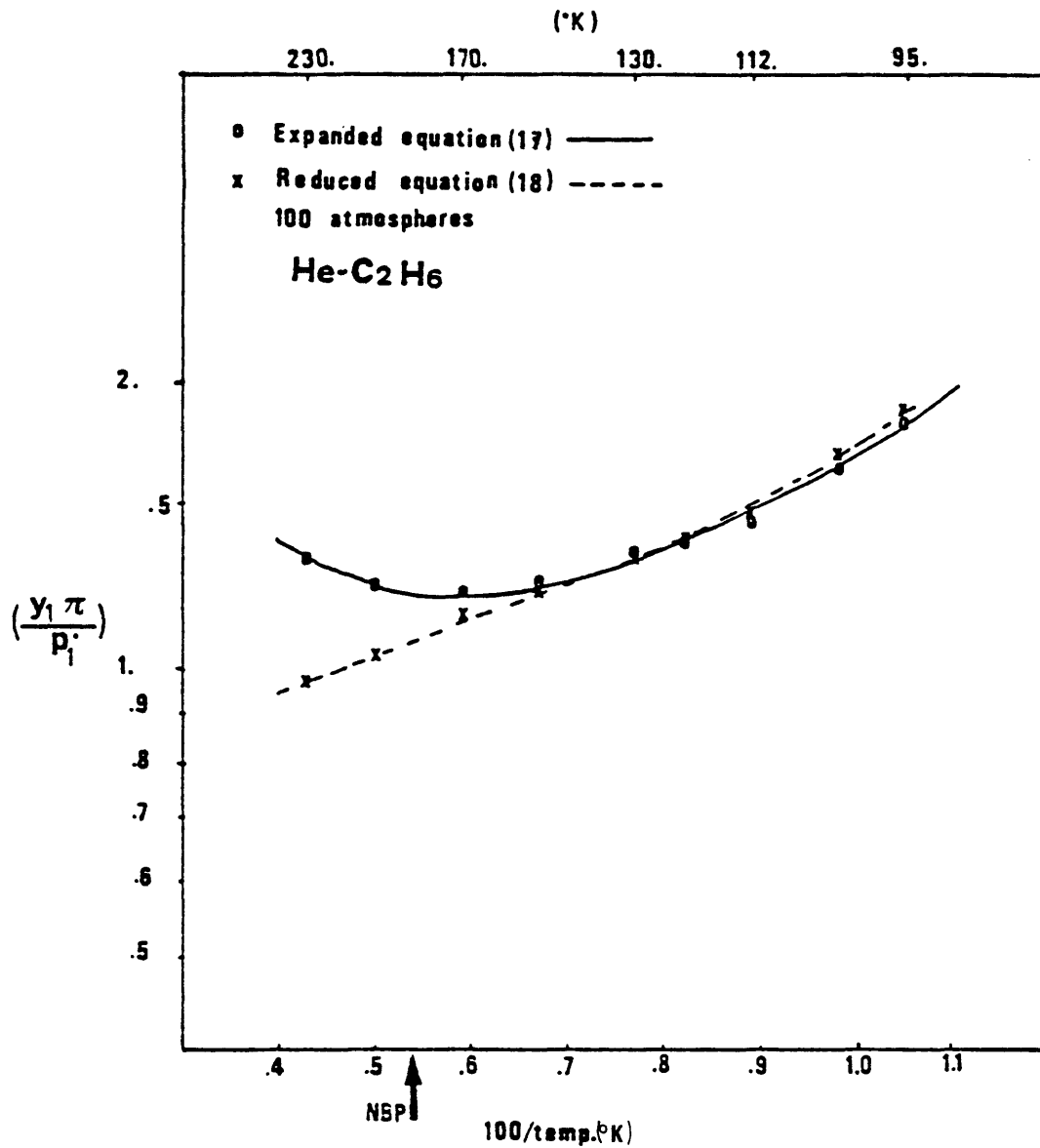
Enhancement Factor at Reciprocal Temperature Using Expanded Equation (17) and Reduced Equation (18) of He-C<sub>2</sub>H<sub>6</sub> System

FIGURE No. 8



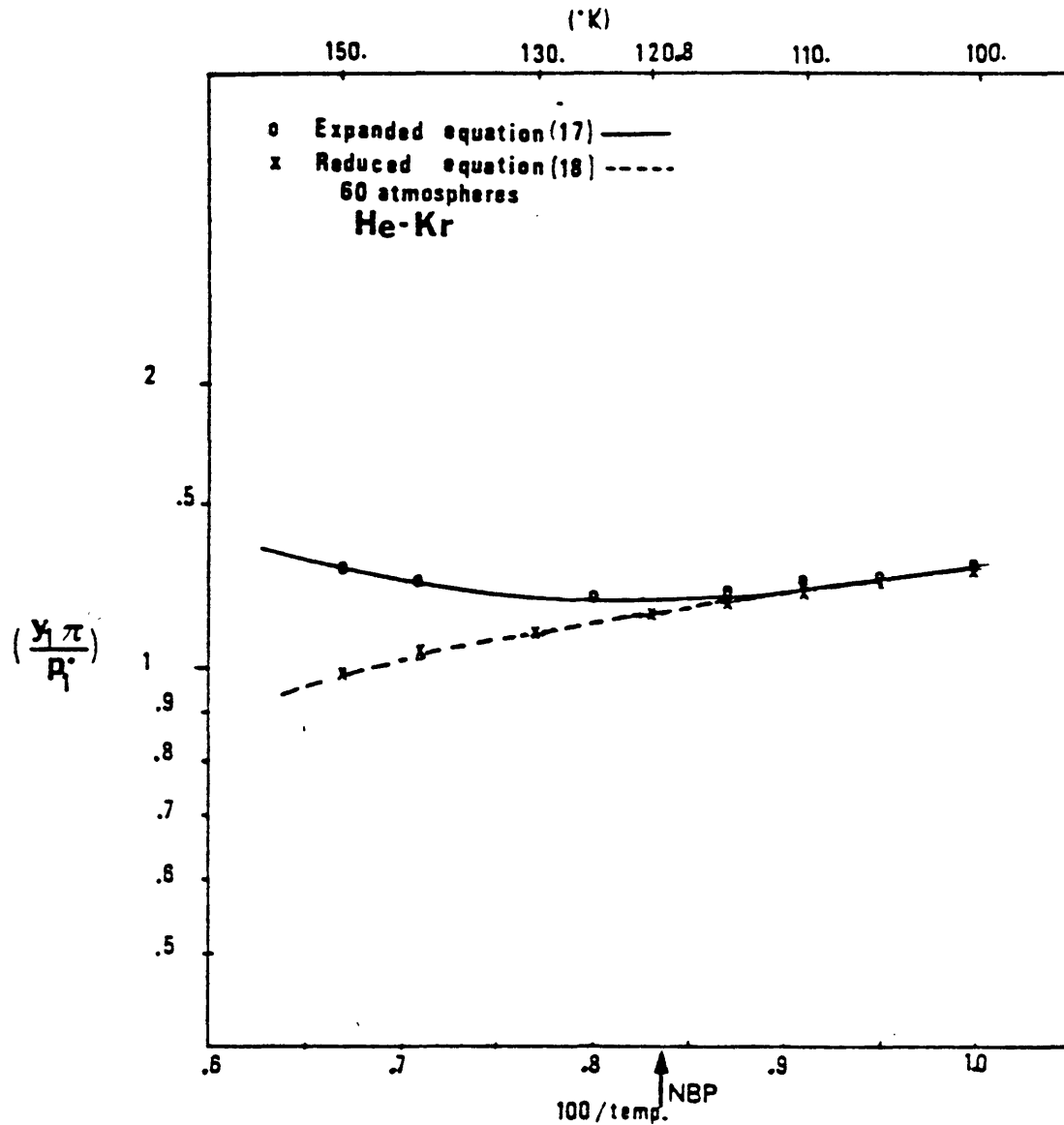
Enhancement Factor at Reciprocal Temperature Using Expanded Equation (17) and Reduced Equation (18) of He-C<sub>2</sub>H<sub>6</sub> System

FIGURE No. 9



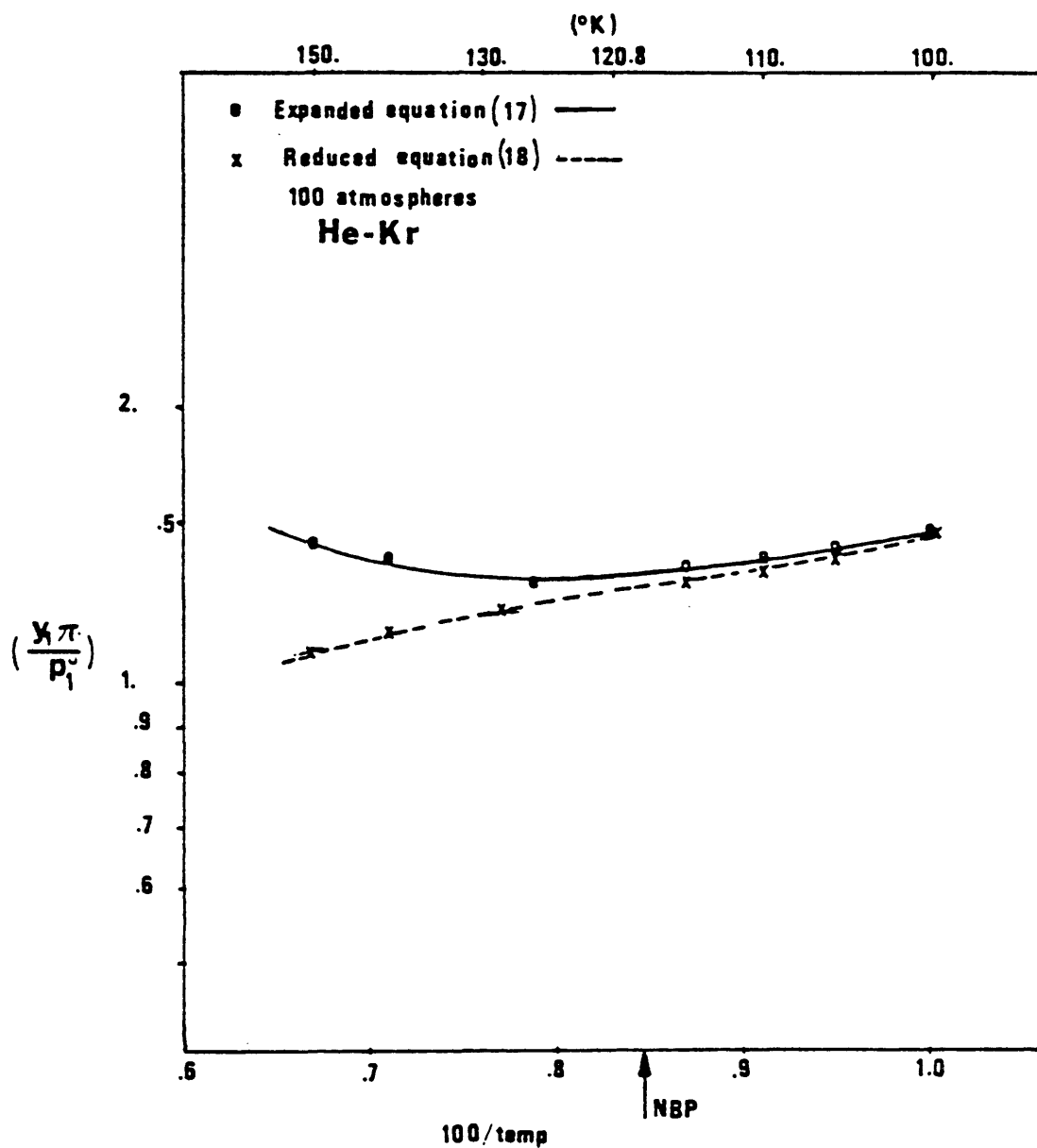
Enhancement Factor at Reciprocal Temperature Using Expanded Equation (17) and Reduced Equation (18) of He-C<sub>2</sub>H<sub>6</sub> System

FIGURE No. 10



Enhancement Factor at Reciprocal Temperature Using Expanded Equation (17) and Reduced Equation (18) of He-Kr System

FIGURE No. 11



Enhancement Factor at Reciprocal Temperature Using Expanded Equation (17) and Reduced Equation (18) of He-Kr System

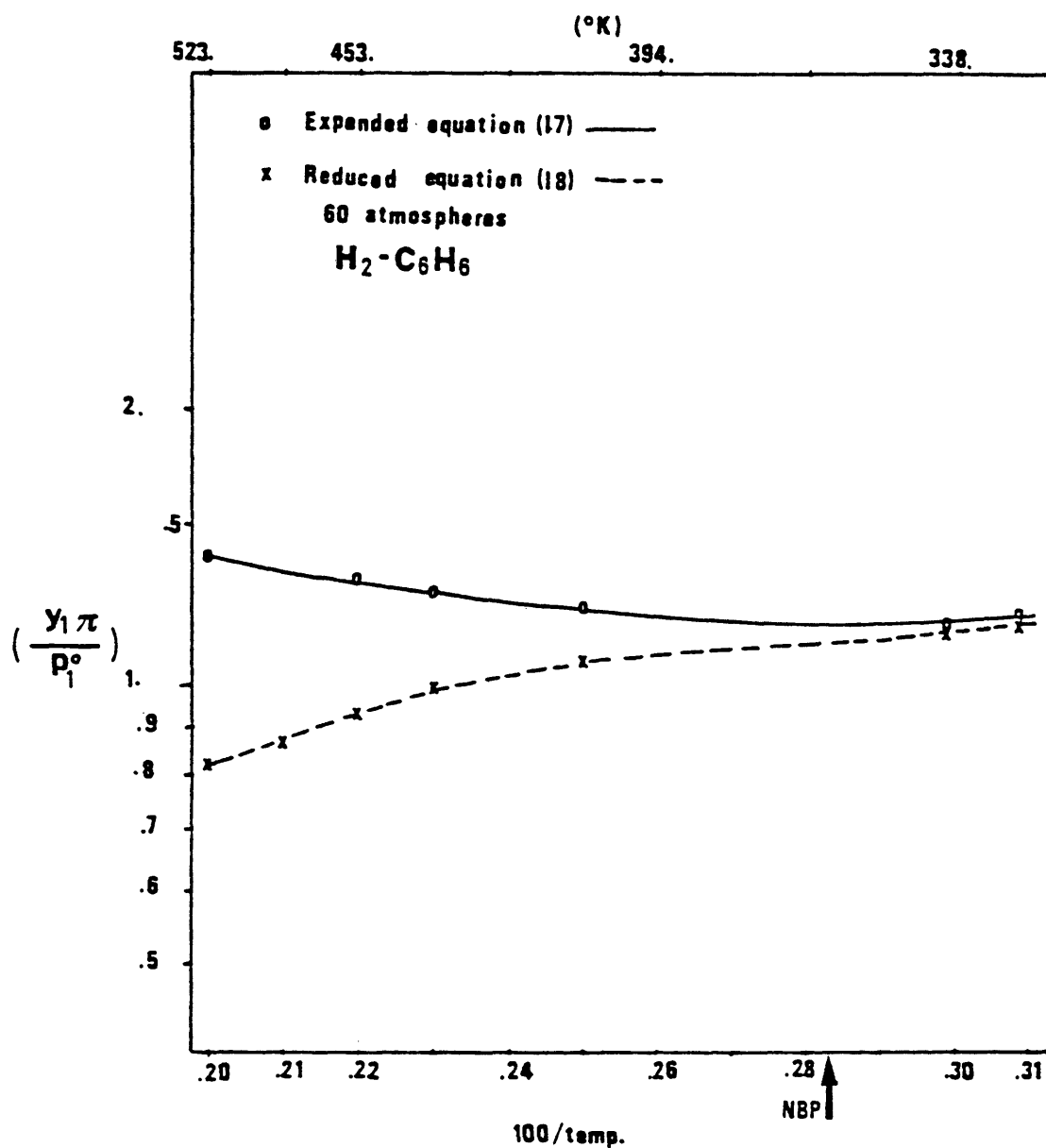
(116.4 °K) while the reduced Equation (18) again predicts no minimum.

The enhancement factors calculated from Equations (17) and (18) for the system  $H_2-C_6H_6$  are shown in Figures 12 and 13 at 60.0 and 100.0 atmospheres. A minimum near the normal boiling point of  $C_6H_6$  is shown in both figures. Few experimental data are available for temperatures below 80.0 °C for the system  $H_2-C_6H_6$ . The data reported by Ipatieff [29], Teodorovitch, Brestkine and Artemovitch were obtained at very high pressures, between 200.0 and 3000.0 atmospheres; the large deviation appearing in the predicted values from their data limit the application to the present study.

A minimum value of enhancement factor of  $H_2-C_2H_6$  is not apparent when the enhancement factor calculated from Equation (17) is plotted against reciprocal temperature (see Figure 14). Nine isotherms of Hiza, Heck and Kidnay [19] and three isotherms of Williams and Katz [20] were used to investigate the existence of a minimum enhancement factor.

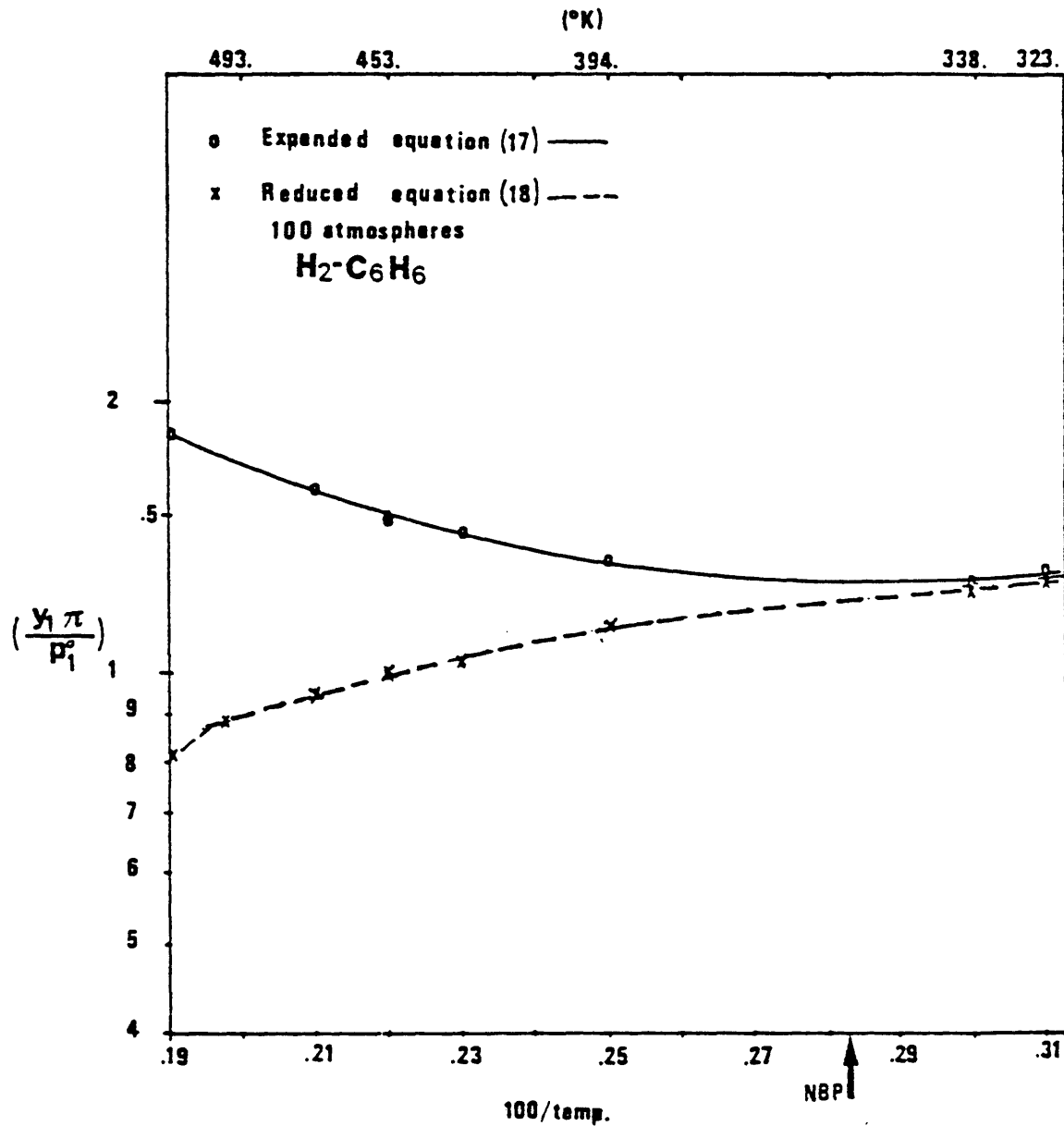
The first step in the determination of the terms that cause a minimum in the enhancement factor predicted by the "expanded equation" was to study the variation of the "Poynting correction", "Phipure" and "Phimixture" with the reciprocal temper-

FIGURE No. 12



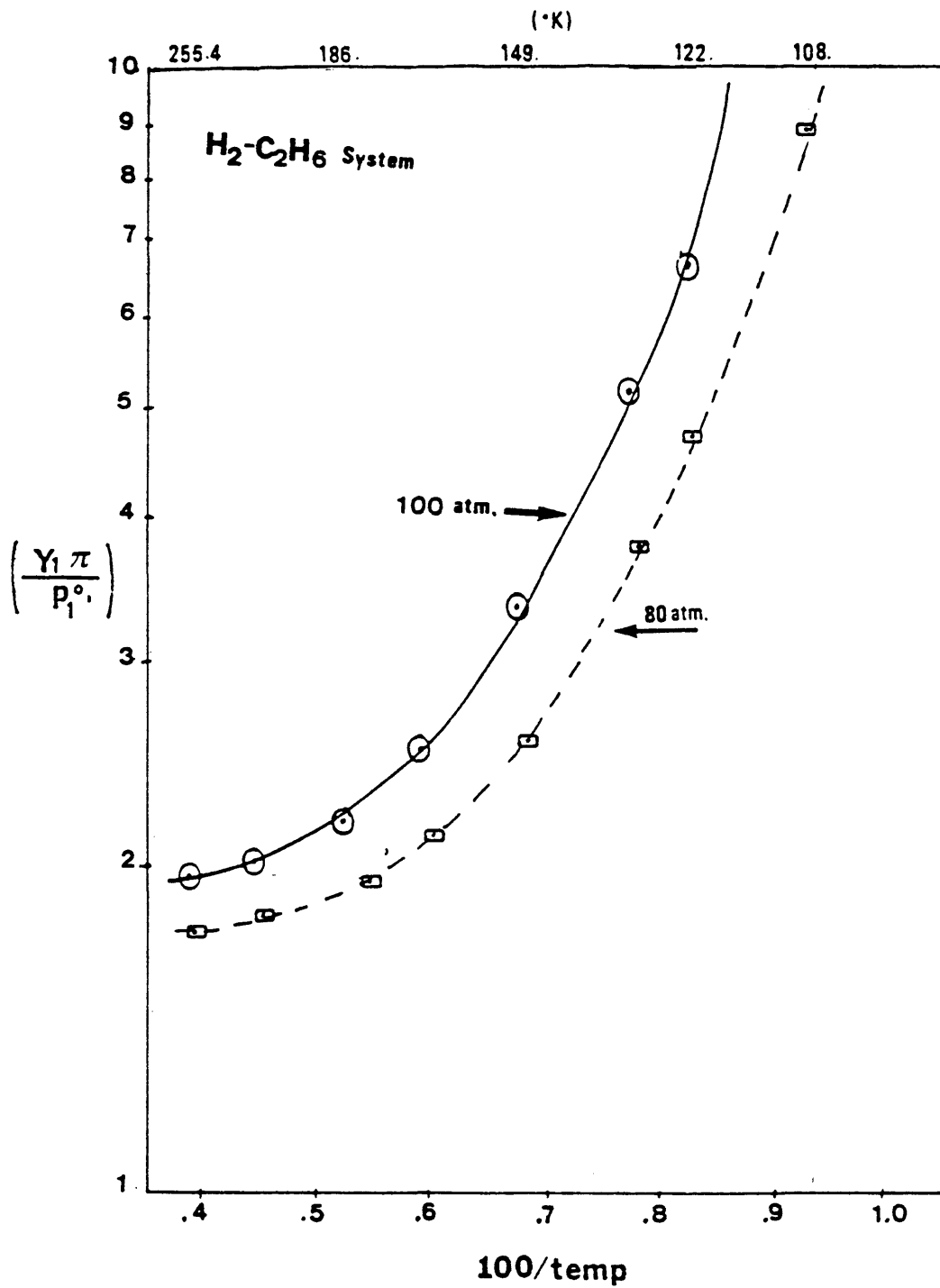
Enhancement Factor at Reciprocal Temperature Using Expanded Equation (17) and Reduced Equation (18) of  $H_2-C_6H_6$  System

FIGURE No. 13



Enhancement Factor at Reciprocal Temperature Using Expanded Equation (17) and Reduced Equation (18) of  $H_2-C_6H_6$  System

FIGURE No. 14

Enhancement Factor at Reciprocal Temperature for H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> System

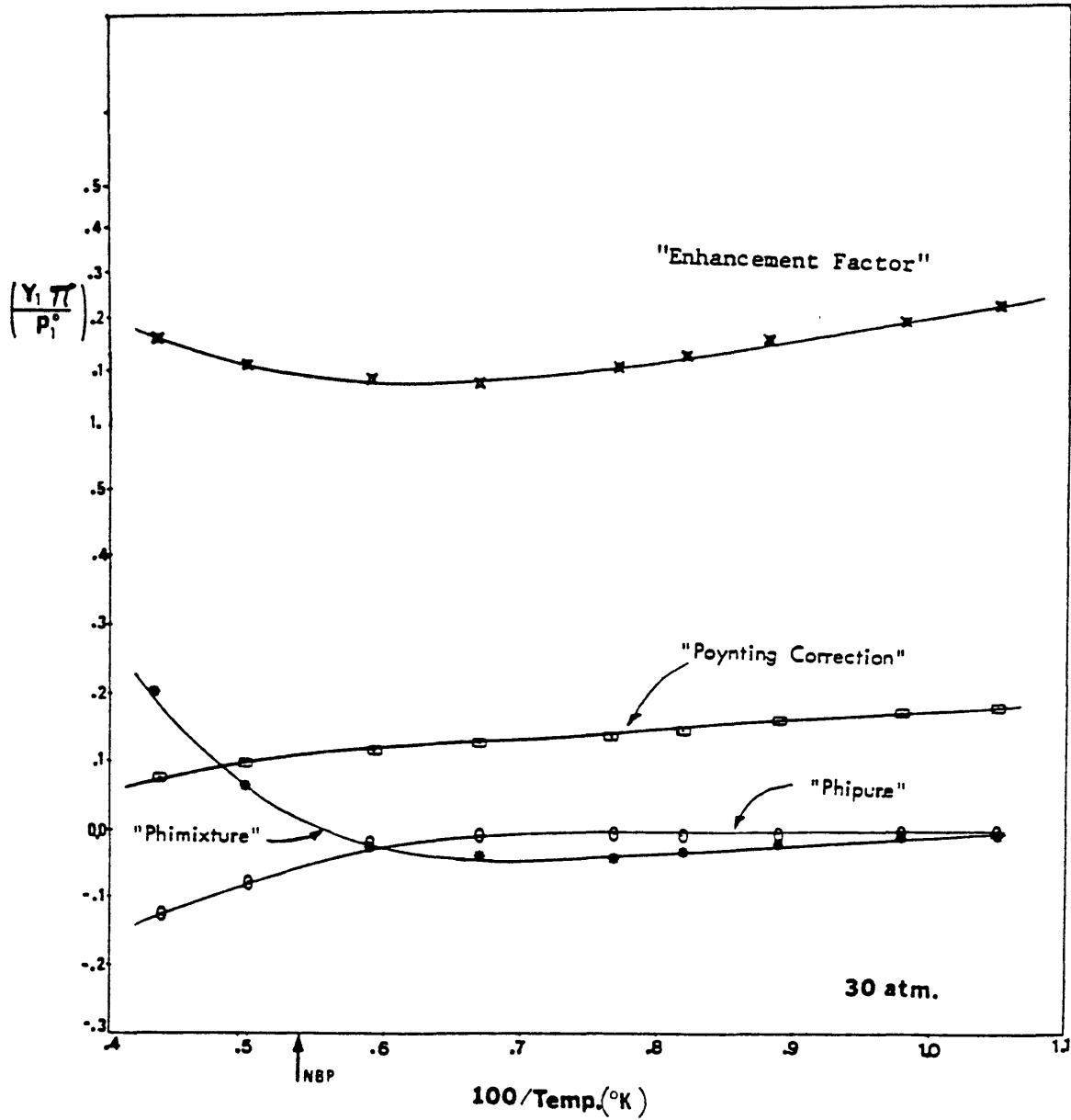
ature. For the He-C<sub>2</sub>H<sub>6</sub> system shown in Figures 15, 16, and 17. The "Poynting correction" and "Phipure" ascend gently and the "Phimixture" term minimizes near the normal boiling of ethane (184.6°K).

The analysis suggests that one or more terms in the "Phimixture" are responsible for minimum enhancement factor. The same analyses mentioned for the He-C<sub>2</sub>H<sub>6</sub> were done for the He-Kr system as shown in Figures 18 and 19. These figures show a similar behavior to the He-C<sub>2</sub>H<sub>6</sub> system.

For the H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> the "Poynting correction, "Phipure" and "Phimixture" were plotted versus the reciprocal temperature and are shown in Figure 20. The "Poynting correction" and "Phipure" have the same behavior as that shown in Figure 17 for the He-C<sub>2</sub>H<sub>6</sub> system. Figure 20 shows that "Phimixture" is curved upward in contrast to the behavior of the He-C<sub>2</sub>H<sub>6</sub> system. This also suggests that the terms that are responsible for the minimum enhancement factor are in "Phimixture".

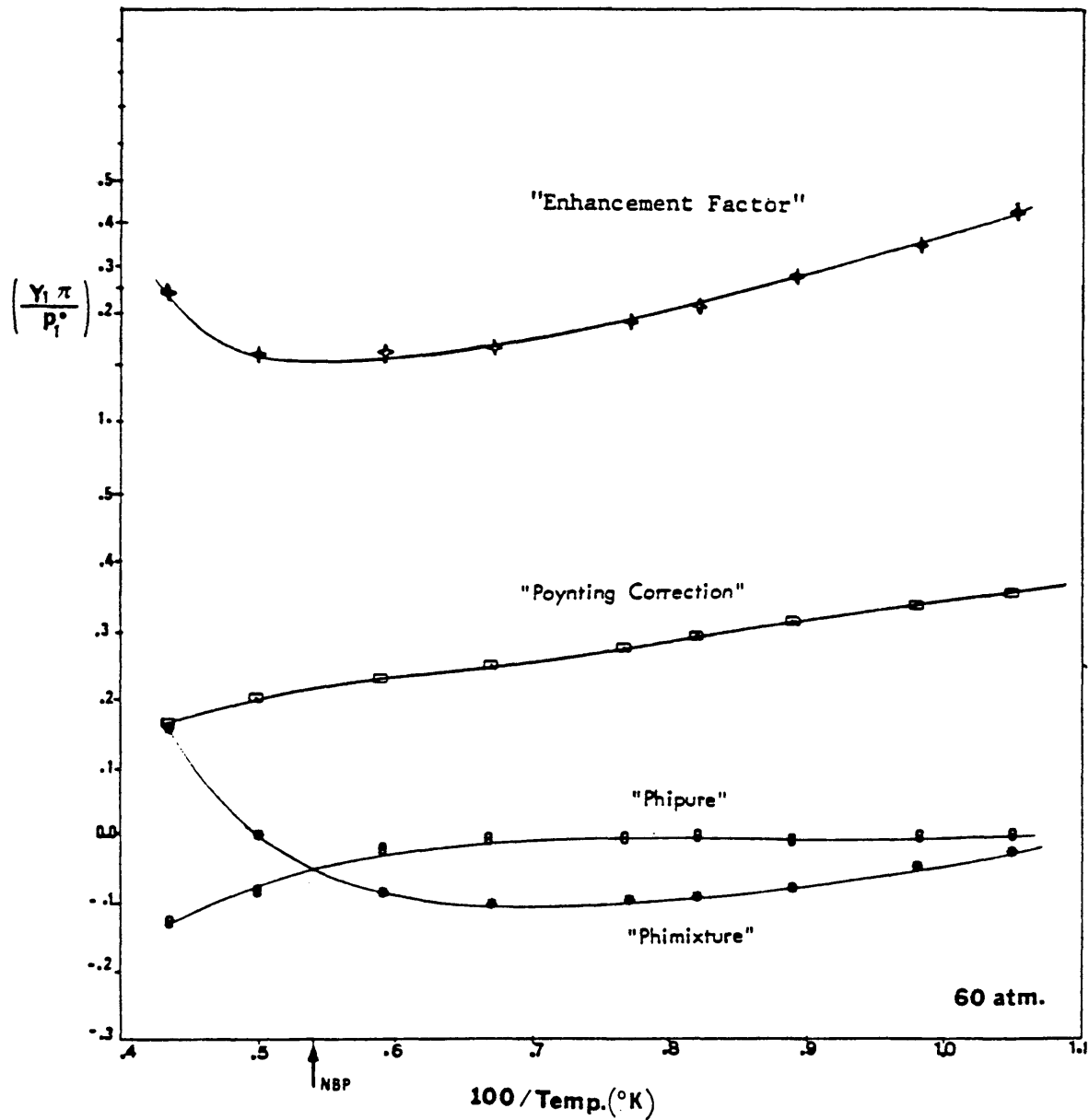
Equation (17) was analyzed in order to find the terms responsible for the minimum enhancement factor. The molar fraction of the light component ( $\gamma_2$ ) was expressed as a function of the molar fraction of the heavy component ( $\gamma_1$ ) applying

FIGURE No. 15



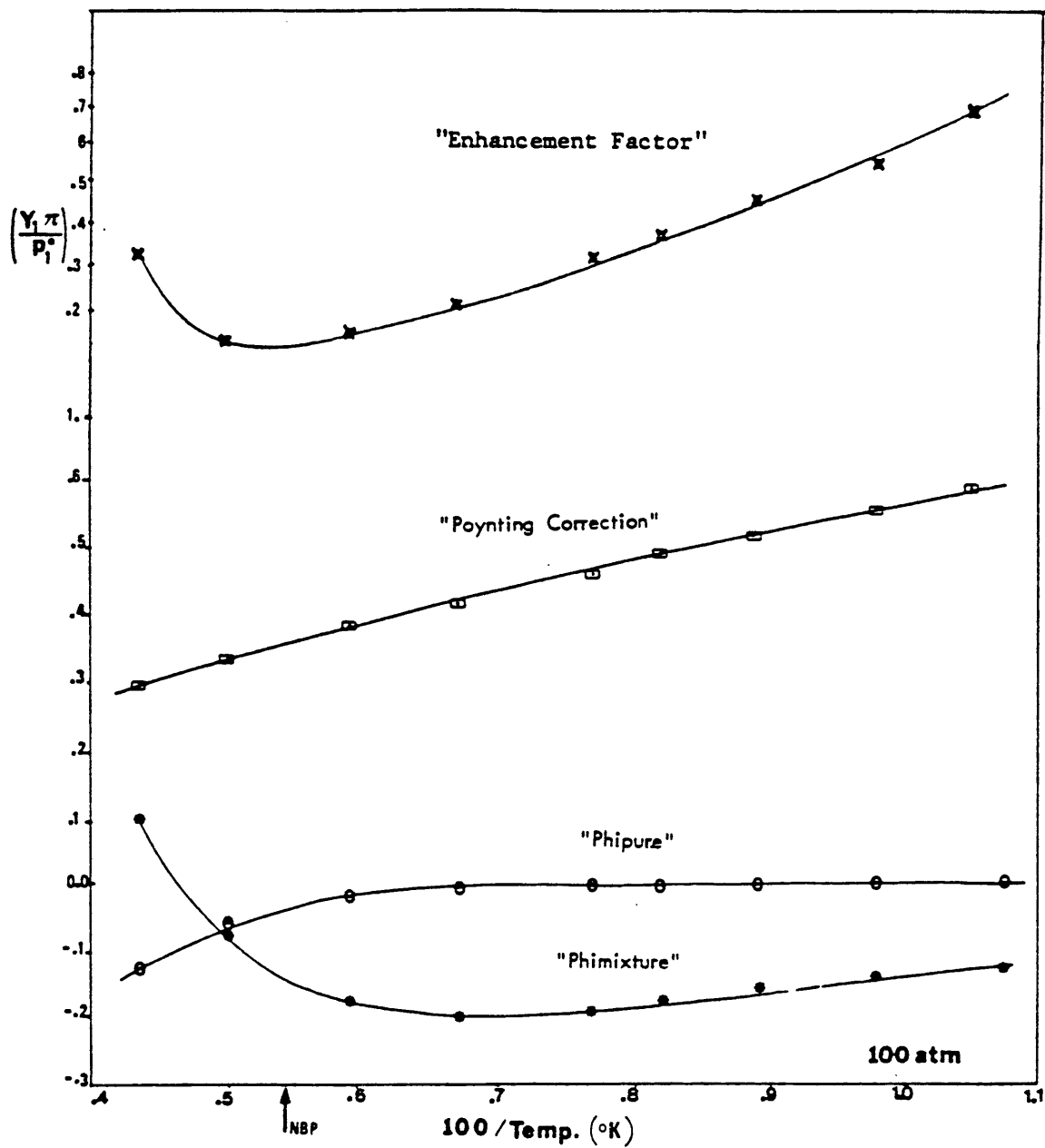
Comparison of "Phimixture", "Phipure", and "Poynting Correction" for He-C<sub>2</sub>H<sub>6</sub> System

FIGURE No. 16



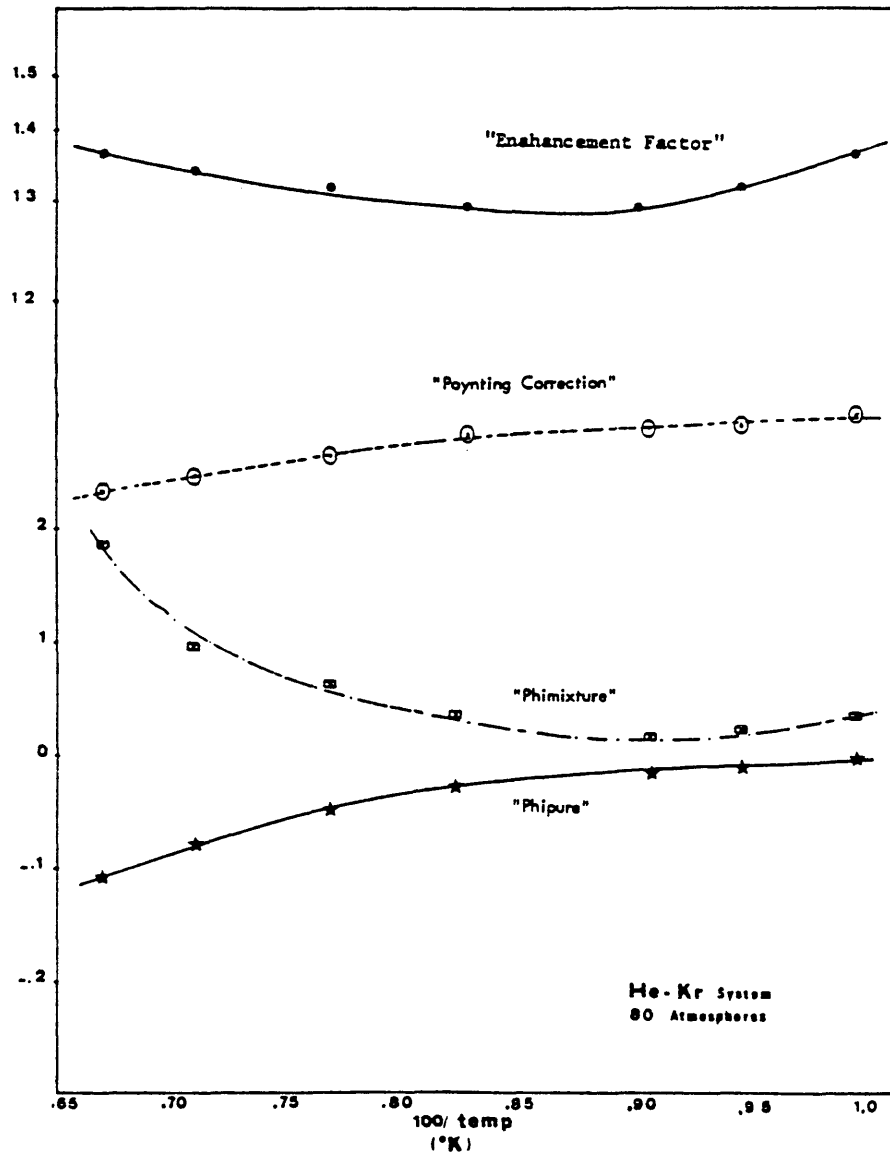
Comparison of "Phimixture", "Phixture", and "Poynting Correction" for He-C<sub>2</sub>H<sub>6</sub> System

FIGURE No. 17



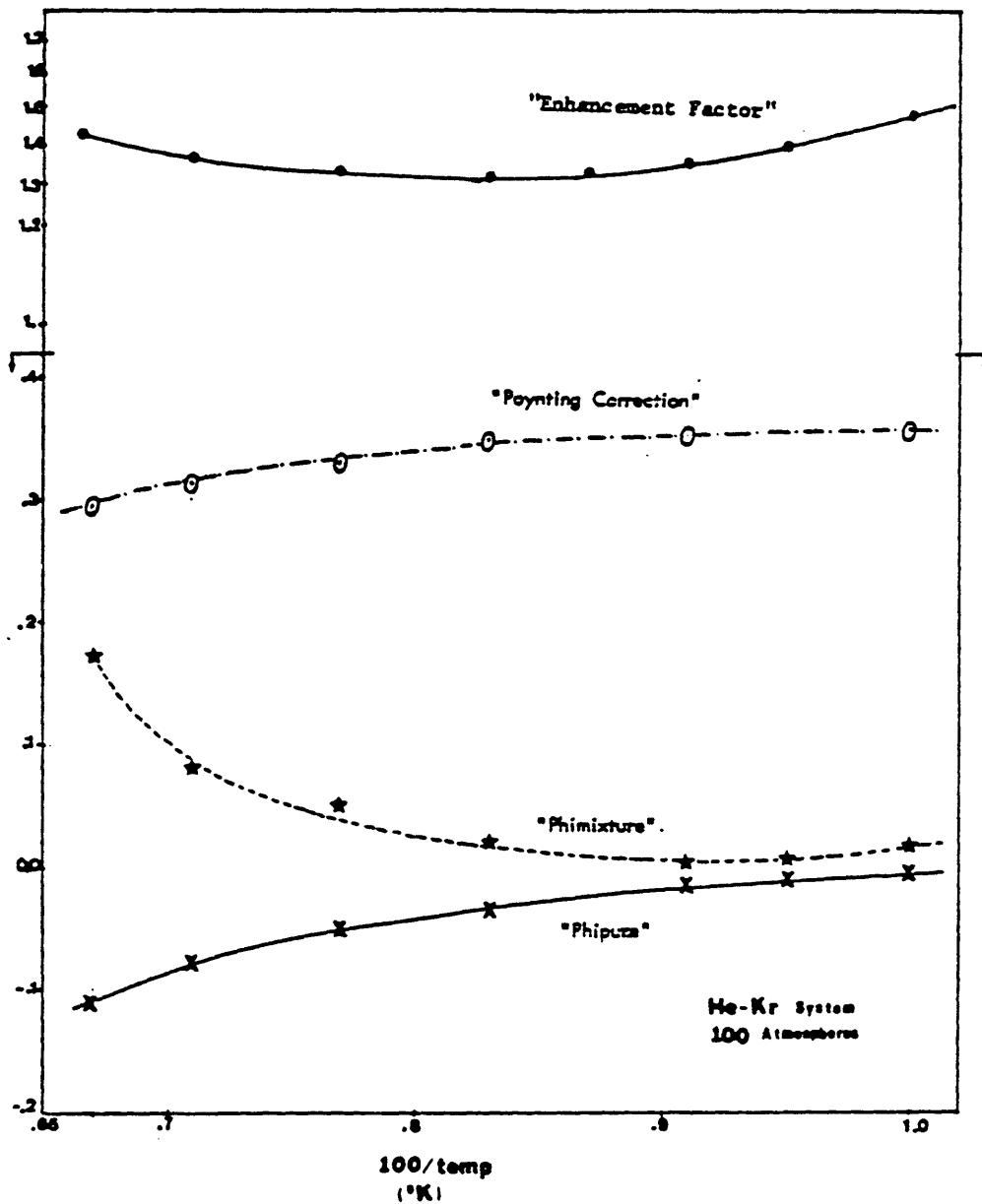
Comparison of "Phimixture", "Phipure", and "Poynting Correction" for He-C<sub>2</sub>H<sub>6</sub> System

FIGURE No. 18



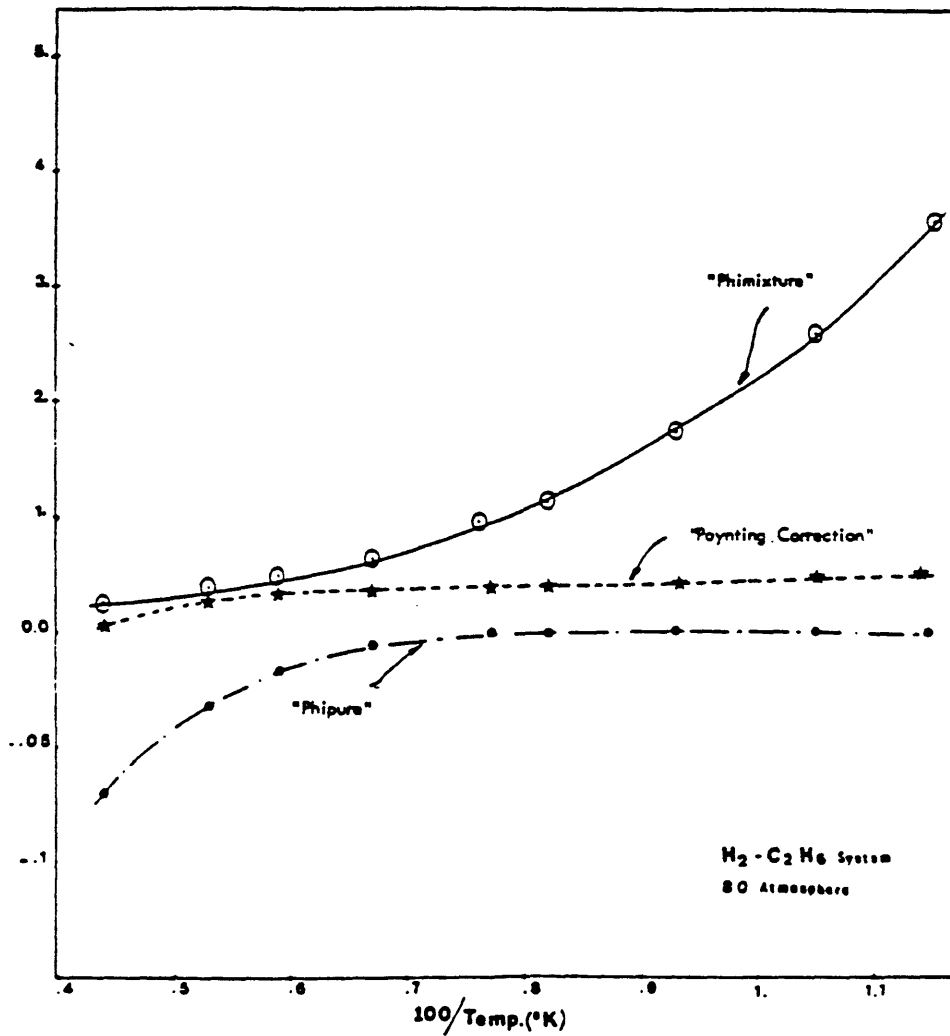
Comparison of "Phimixture", "Phipure", and "Poynting Correction" for He-Kr System

FIGURE No. 19



Comparison of "Phimixture", "Phipure", and "Poynting Correction" for He-Kr System

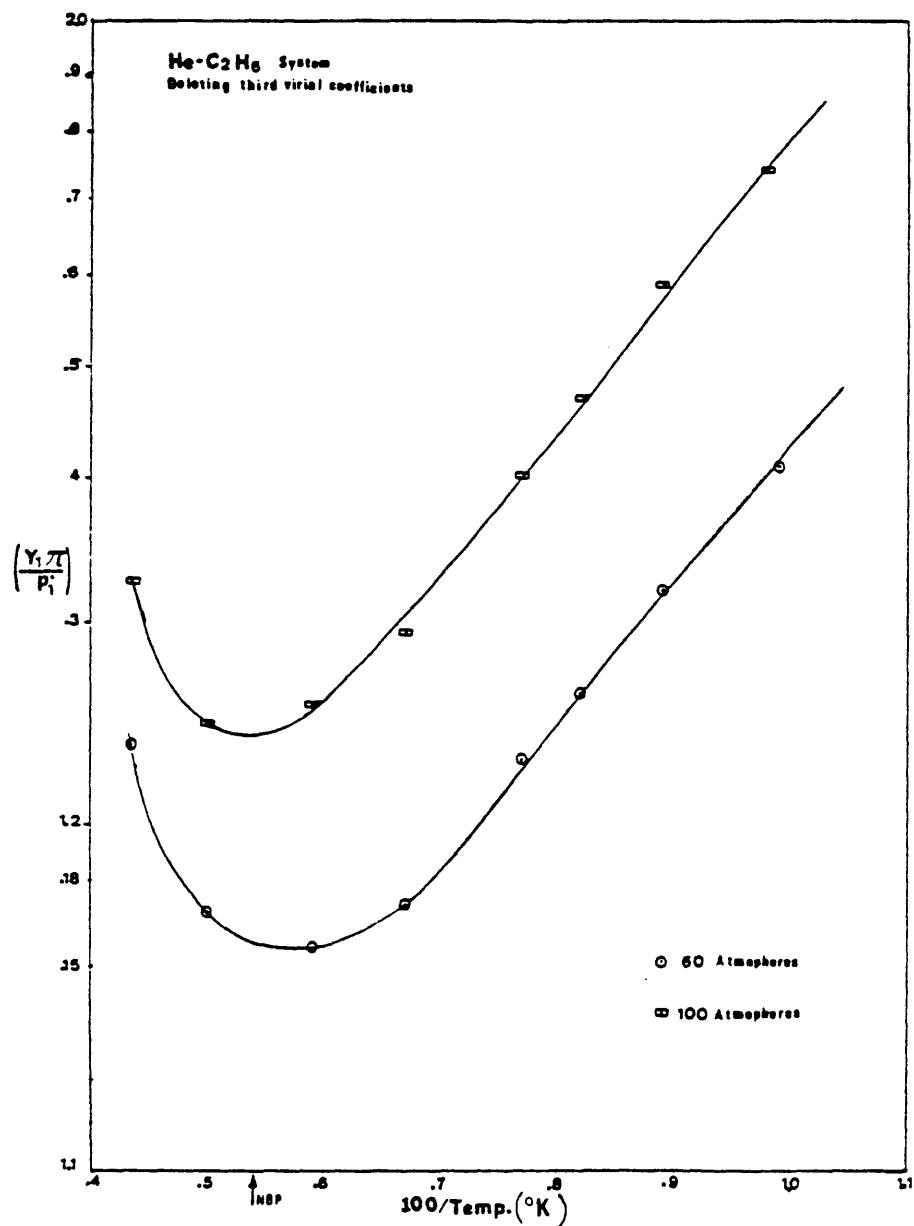
FIGURE No. 20

Comparison of "Phimixture", "Phipure", and "Poynting Correction" for  $H_2-C_2H_6$  System

the equation  $Y_2 = 1 - Y_1$ .

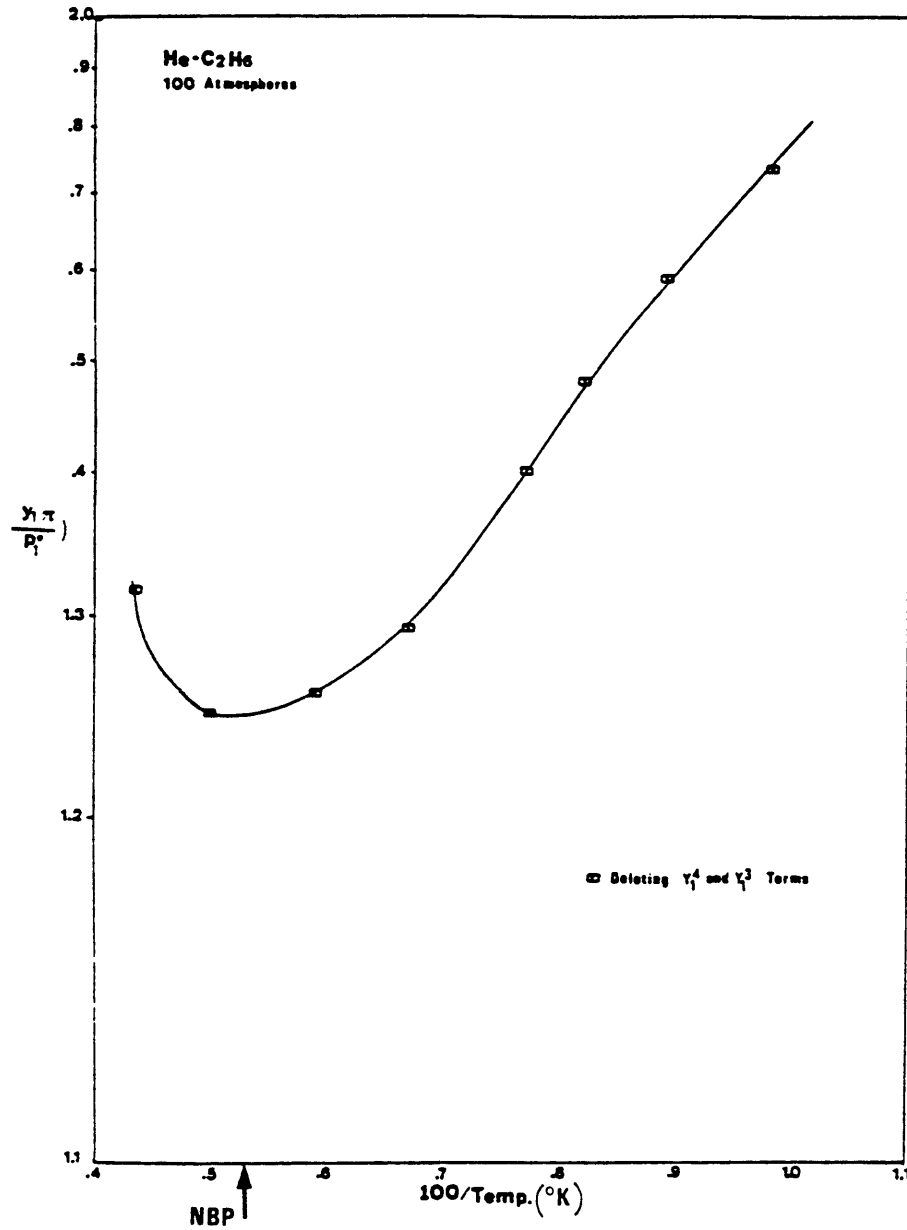
The first set of terms deleted from equation (17) were the terms carrying the third virial coefficients. The enhancement factor versus reciprocal temperature are plotted in the figure 21 at a pressure of 100.0 and 60.0 atmosphere for the He-C<sub>2</sub>H<sub>6</sub> system. The minimum enhancement factor still appears. In continuing this truncation procedure for the terms carrying  $Y_1^4$  and  $Y_1^3$  in the "expanded equation" (17) were deleted; the enhancement factor still shows a minimum with respect to the reciprocal temperature as in Figure 22 at 100.0 atmosphere. Figure 23 shows that the minimum enhancement factor versus reciprocal temperature remains even after dropping the terms with  $Y_1^2$ . The minimum disappears when the terms with  $Y_1$  are removed from the "Expanded equation" (17). In order to investigate which term with  $Y_1$  is responsible for the minimum, all the terms with  $Y_1$  were deleted one at a time. Figure 24 shows the results obtained after dropping all the terms with  $Y_1$  except the term  $2Y_1 B_{11} \pi / RT$ . Therefore the term responsible of the minimum is  $(1 - Y_2^2) B_{11} \pi / RT$  or  $(2Y_1 - Y_1^2) B_{11} \pi / RT$  when  $Y_2$  is expressed as a function of  $Y_1$ . In order to test this conclusion the term  $(2Y_1 - Y_1^2) B_{11} \pi / RT$  was deleted for the He-C<sub>2</sub>H<sub>6</sub>, He-Kr and H<sub>2</sub>-C<sub>6</sub>H<sub>6</sub> systems (see figure 25,26

FIGURE No. 21



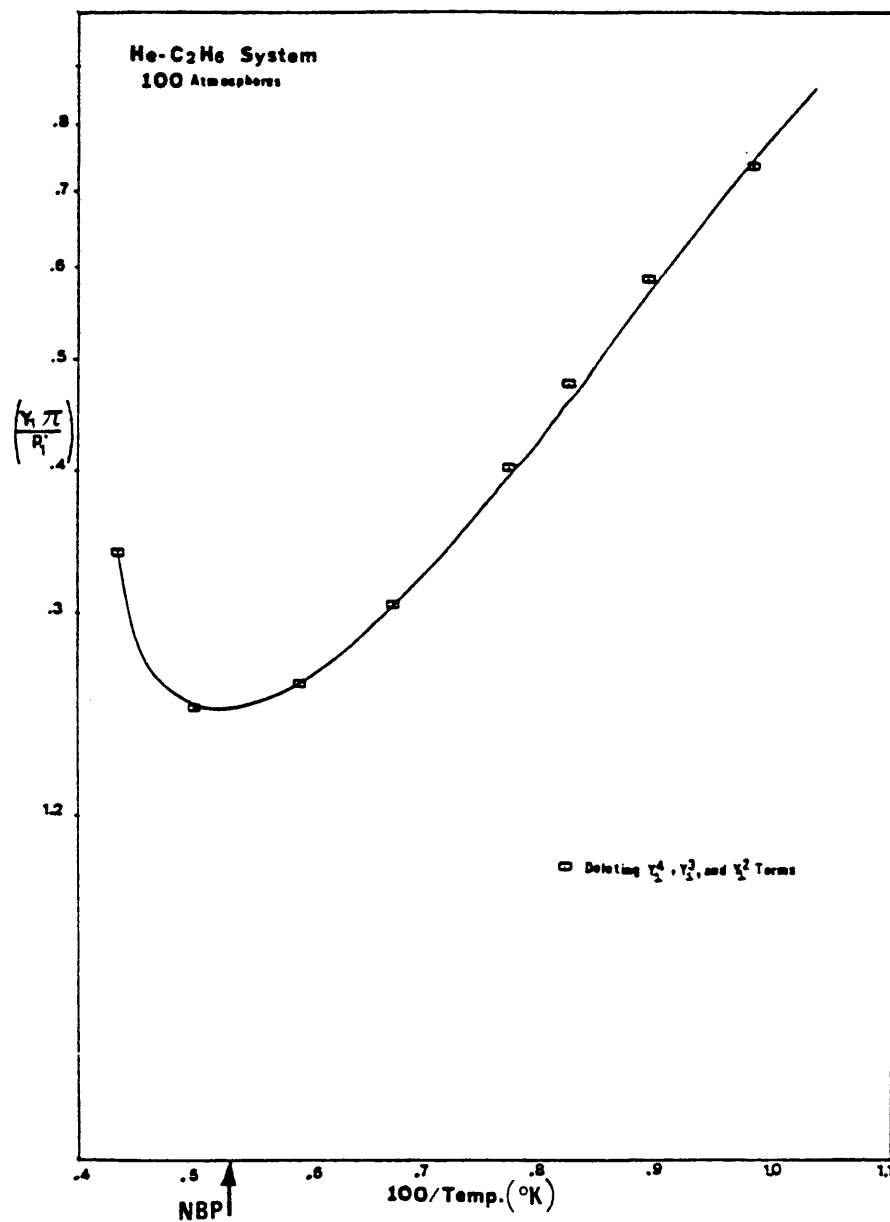
Enhancement Factor at Reciprocal Temperature Deleting Third Virial Coefficients

FIGURE No. 22



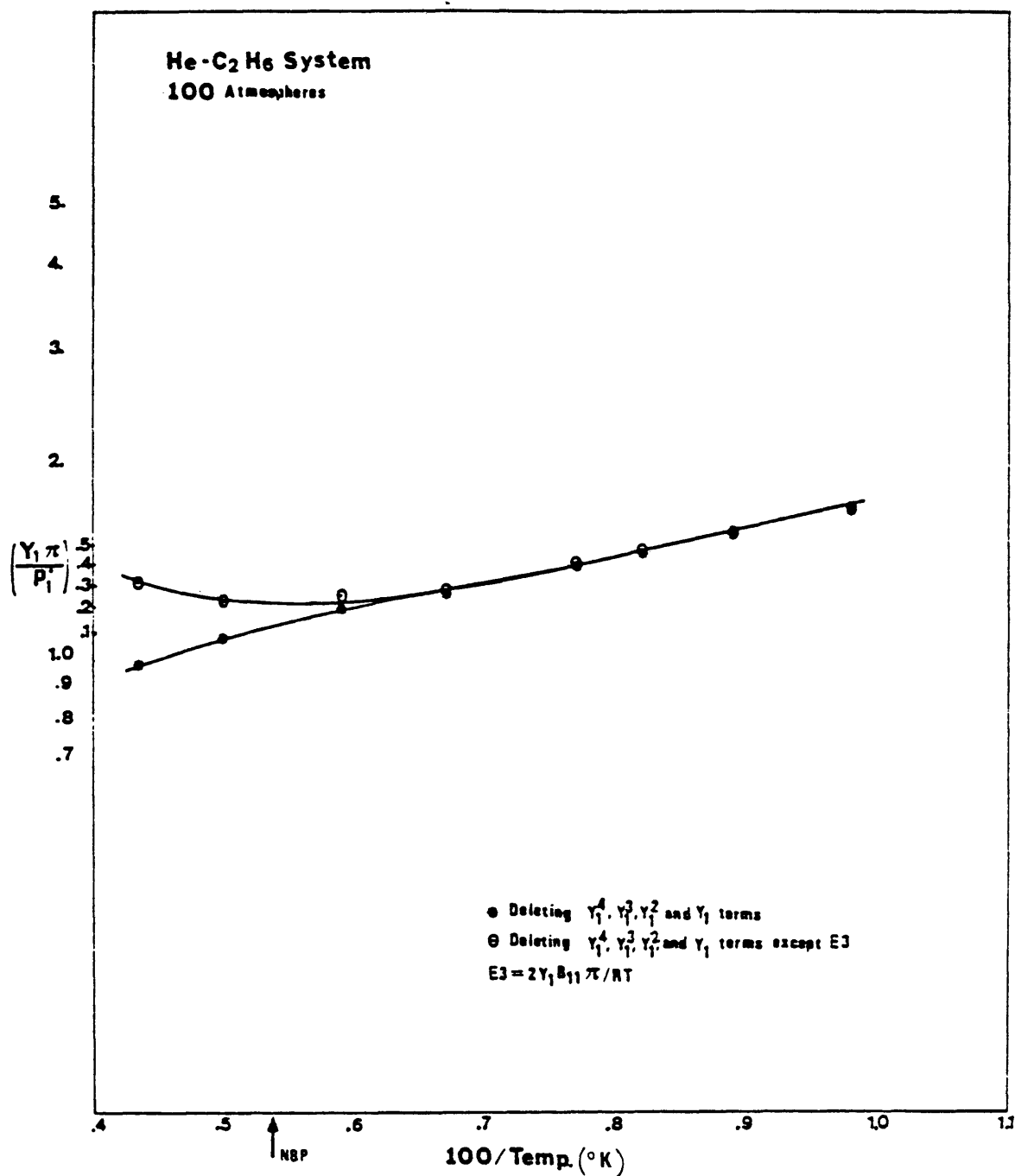
Enhancement Factor at Reciprocal Temperature Deleting  $Y_1^4$  and  $Y_1^3$  Terms

FIGURE No. 23



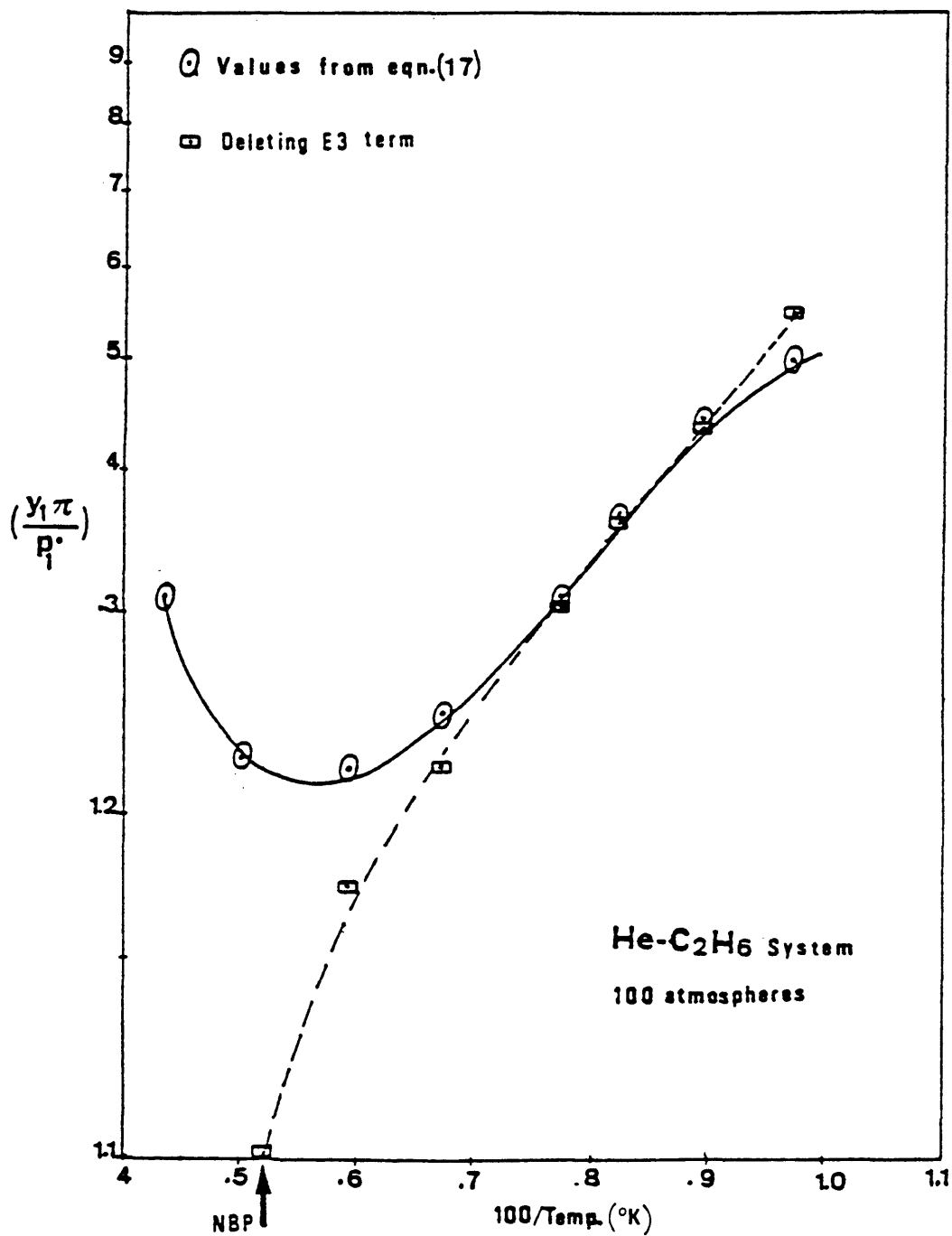
Enhancement Factor at reciprocal Temperature Deleting  $Y_1^4$ ,  $Y_1^3$ ,  
and  $Y_1^2$  Terms

FIGURE No. 24



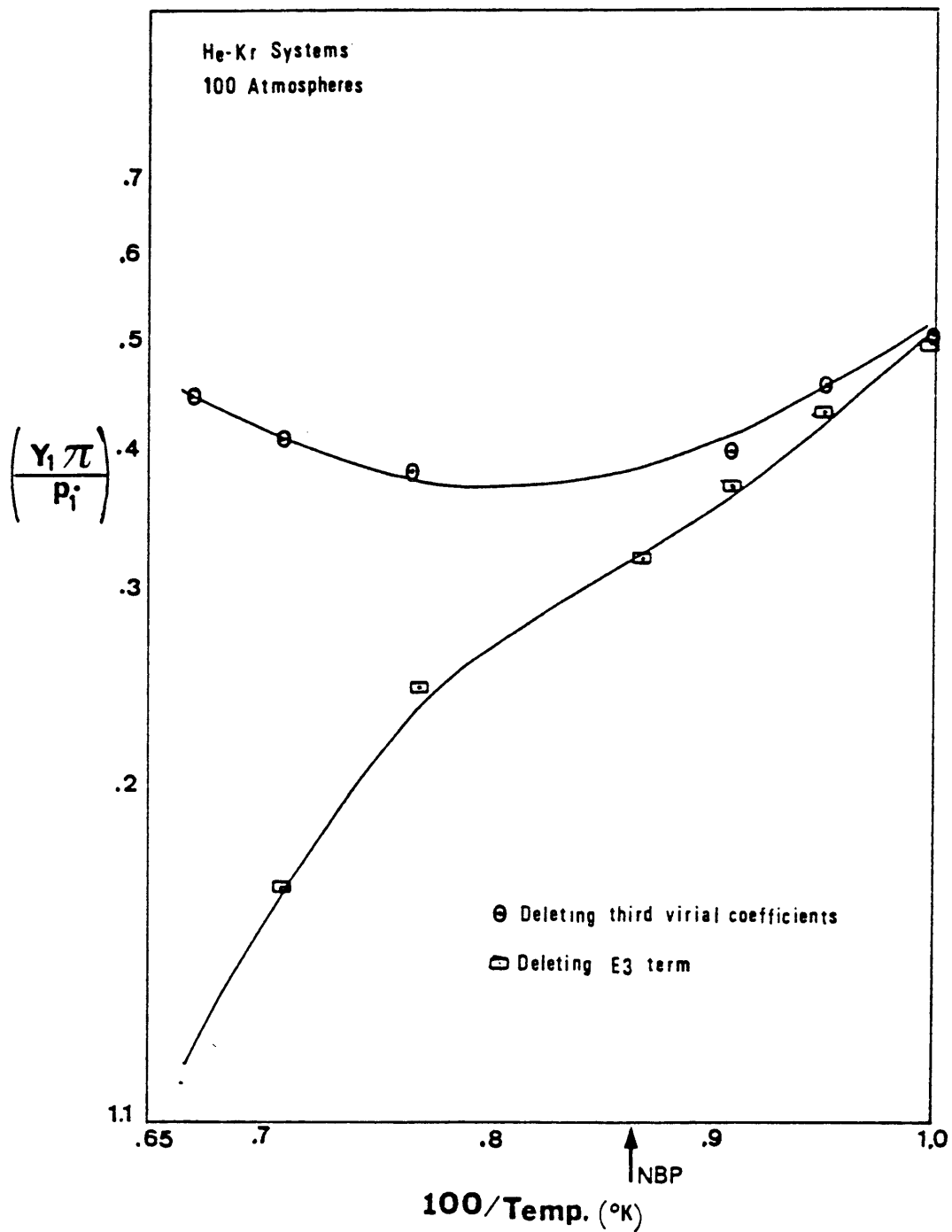
Enhancement Factor at Reciprocal Temperature Deleting all the Terms with  $Y_1$  Except the Term  $2Y_1 B_{11} \pi / RT$

FIGURE No. 25



Enhancement Factor Versus Reciprocal Temperature in the He-C<sub>2</sub>H<sub>6</sub> System from Equation (17) with and without E3 Term

FIGURE No.26



Enhancement Factor Versus Reciprocal Temperature in the He-Kr System Deleting Third Virial Coefficients and E3 Term

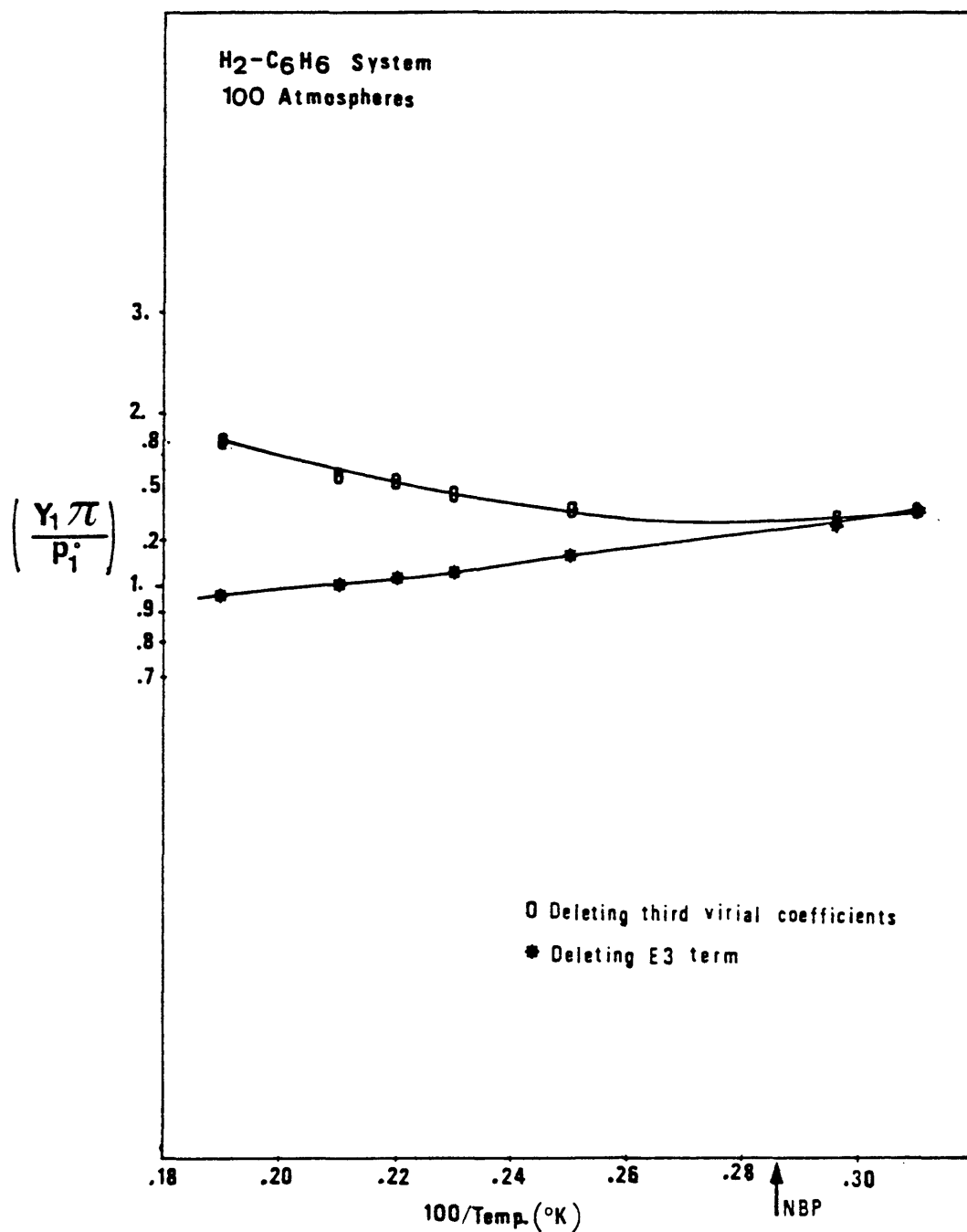
and 27 respectively). The minimum of the enhancement factor for those systems dissappeared in all cases.

Other important analyses for the He-C<sub>2</sub>H<sub>6</sub> and H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> was carried out. The values of "Phimixture" in the He-C<sub>2</sub>H<sub>6</sub> from the "expanded equation (17) without the term  $(1 - Y_2^2) B_{11} \pi / RT$  were plotted against reciprocal temperature (see Figures 28 and 29) at pressure of 60.0 and 100.0 atmospheres. Clearly these plots show that the difference between "Phimixture" in the "Reduced" equation and that without the term  $(1 - Y_2^2) B_{11} \pi / RT$  in the "expanded" equation doesn't show a significant difference.

Figure 30 shows the effect of the values of "Phimixture" of the "expanded equation" (17) and that without  $(1 - Y_2^2) B_{11} \pi / RT$  terms for the H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> system do not show a significant difference.

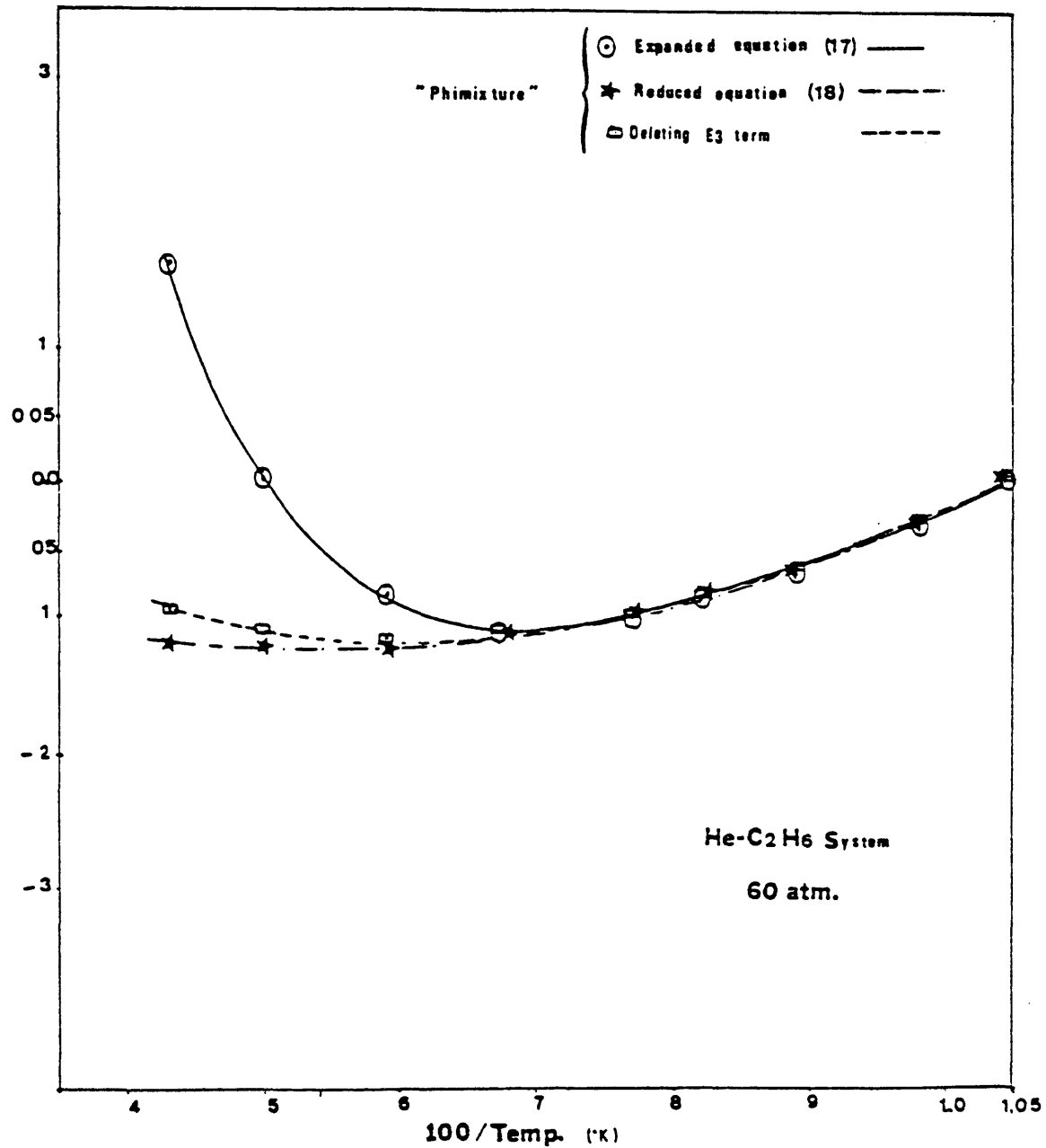
The enhancement factor for the H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> with the  $(1 - Y_2^2) B_{11} \pi / RT$  and without this term were plotted against reciprocal temperature, these two plots do not show a significant difference. (figure 31). This doesn't hold for He-C<sub>2</sub>H<sub>6</sub> system which is evident in the Figure 25. In general this analysis shows that term  $(1 - Y_2^2) B_{11} \pi / RT$  has a remarkable influence for the existence of the minimum enhancement factor.

FIGURE No. 27



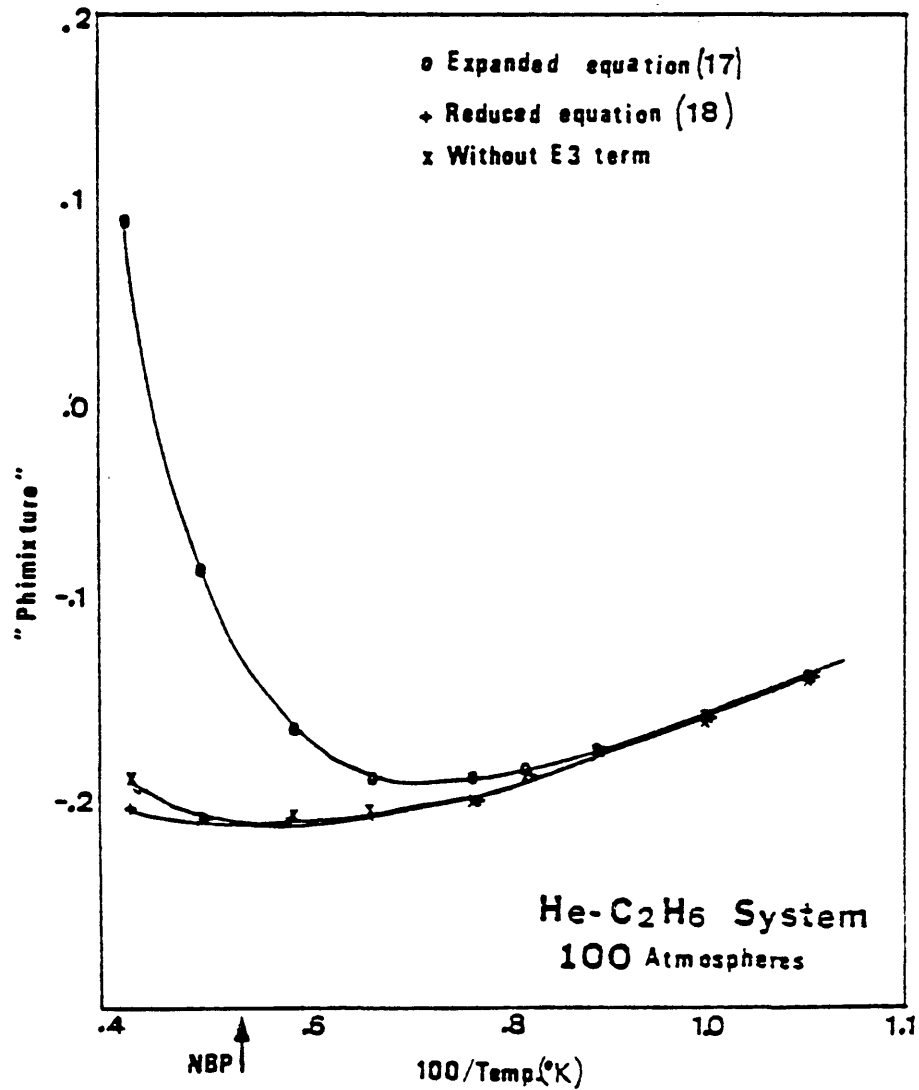
Enhancement Factor Versus Reciprocal Temperature in the H<sub>2</sub>-C<sub>6</sub>H<sub>6</sub> System Deleting Third Virial Coefficients and E3 Term

FIGURE No. 28



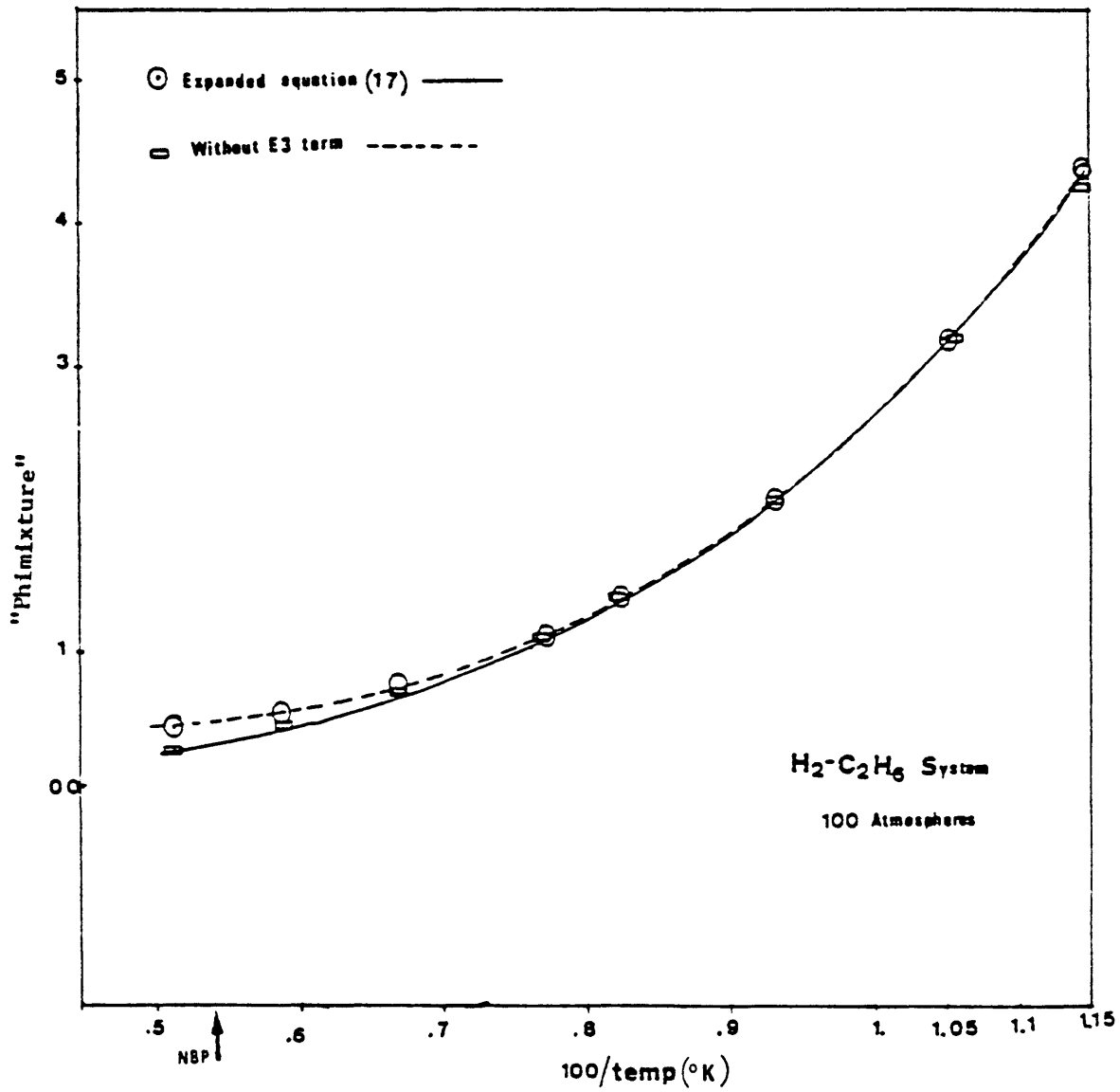
Plot of "Phimixture" for the He-C<sub>2</sub>H<sub>6</sub> System from Equation (18), and Equation (17) with and without E3 Term

FIGURE No. 29



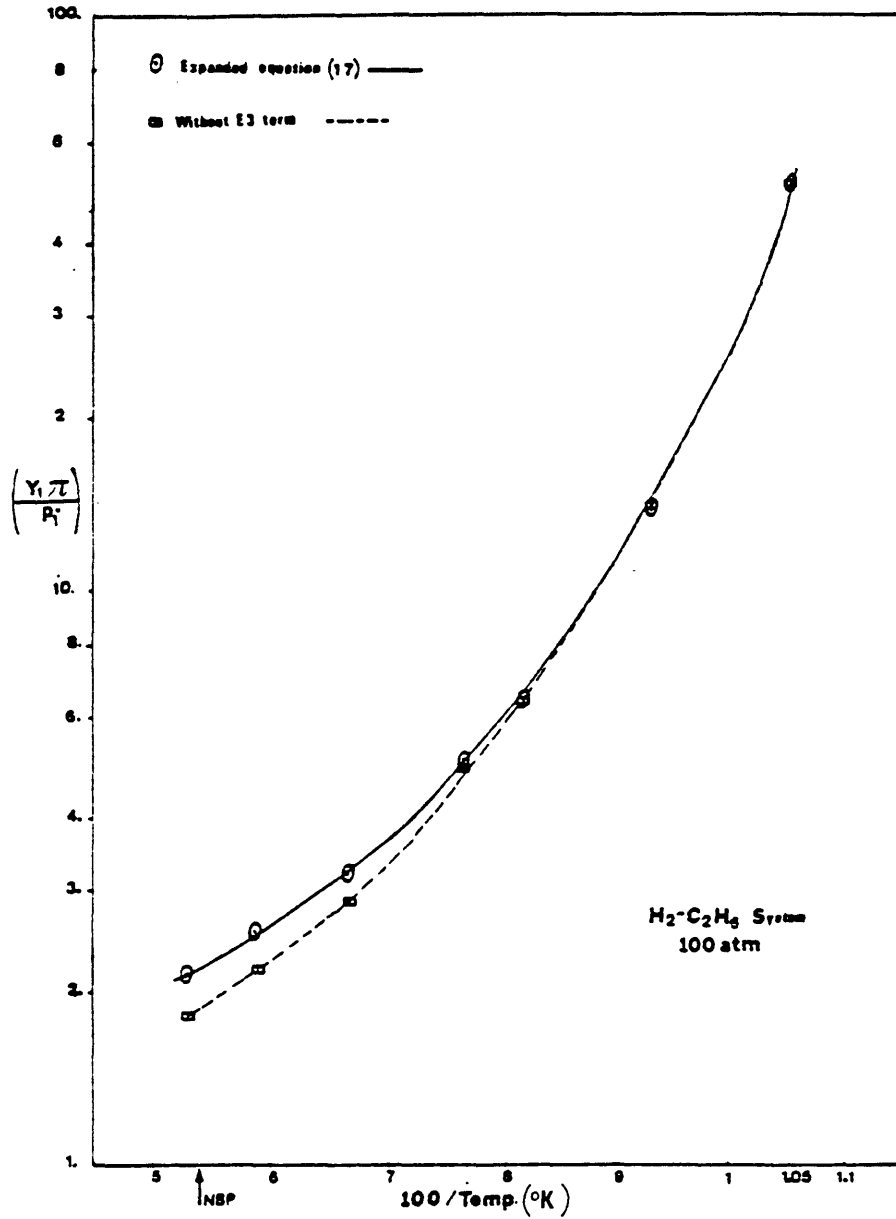
Plot of "Phimixture" in the He-C<sub>2</sub>H<sub>6</sub> System Using Equation (18), and Equation (17) with and without E3 Term

FIGURE No 30



Plot of "Phimixture" in the H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> System Using Equation (17) with and without E3 Term

FIGURE No. 31



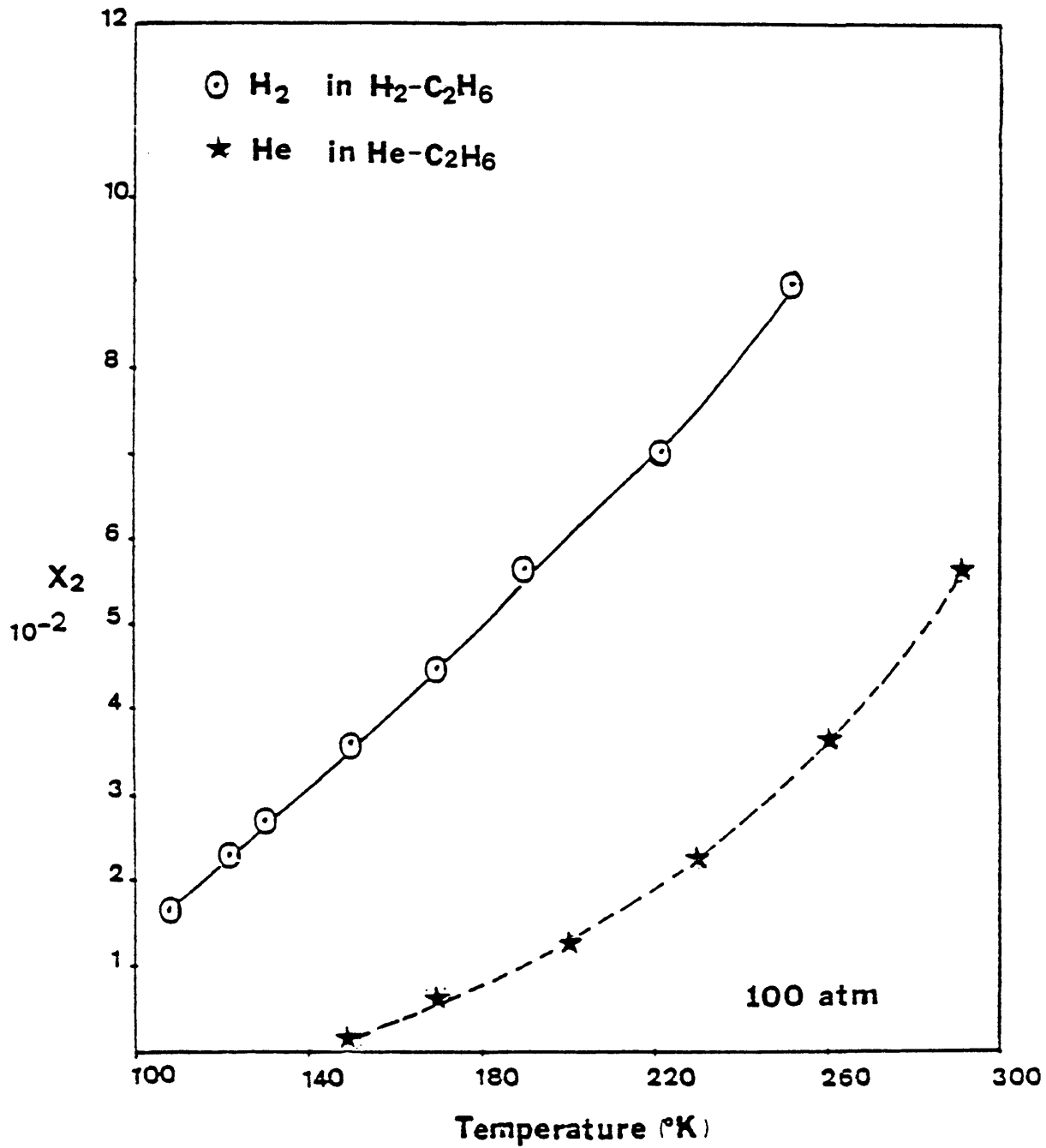
Enhancement Factor in the H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> System Versus Reciprocal Temperature Using Equation (17) with and without E3 Term

The mole fraction of the light components in liquid phase ( $X_2$ ) were plotted against reciprocal temperature (see Figure 32) in looking for an answer for the existence of the minimum enhancement factor for the systems He-C<sub>2</sub>H<sub>6</sub> and H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> due to the solubility effects. This figure shows the high solubility of H<sub>2</sub> over He and doesn't show a minimum or maximum. Some systems such as CH<sub>4</sub>-n-C<sub>7</sub>H<sub>16</sub> shown in Figure 33, show a minimum in enhancement factor closely follow a minimization in solubility. Figure 32 indicates that the solubility of the light component alone does not cause the enhancement factor minimization.

In search of relationship between the solubility of gases and minimum enhancement factor, a plot of the molar fraction of the heavy component versus reciprocal reduced temperature was made. This reduced temperature was calculated by  $T_r = T / T_{Cij}$ . The critical temperature for the light component were calculated by the method of Chueh and Prausnitz [7] using equation (28).

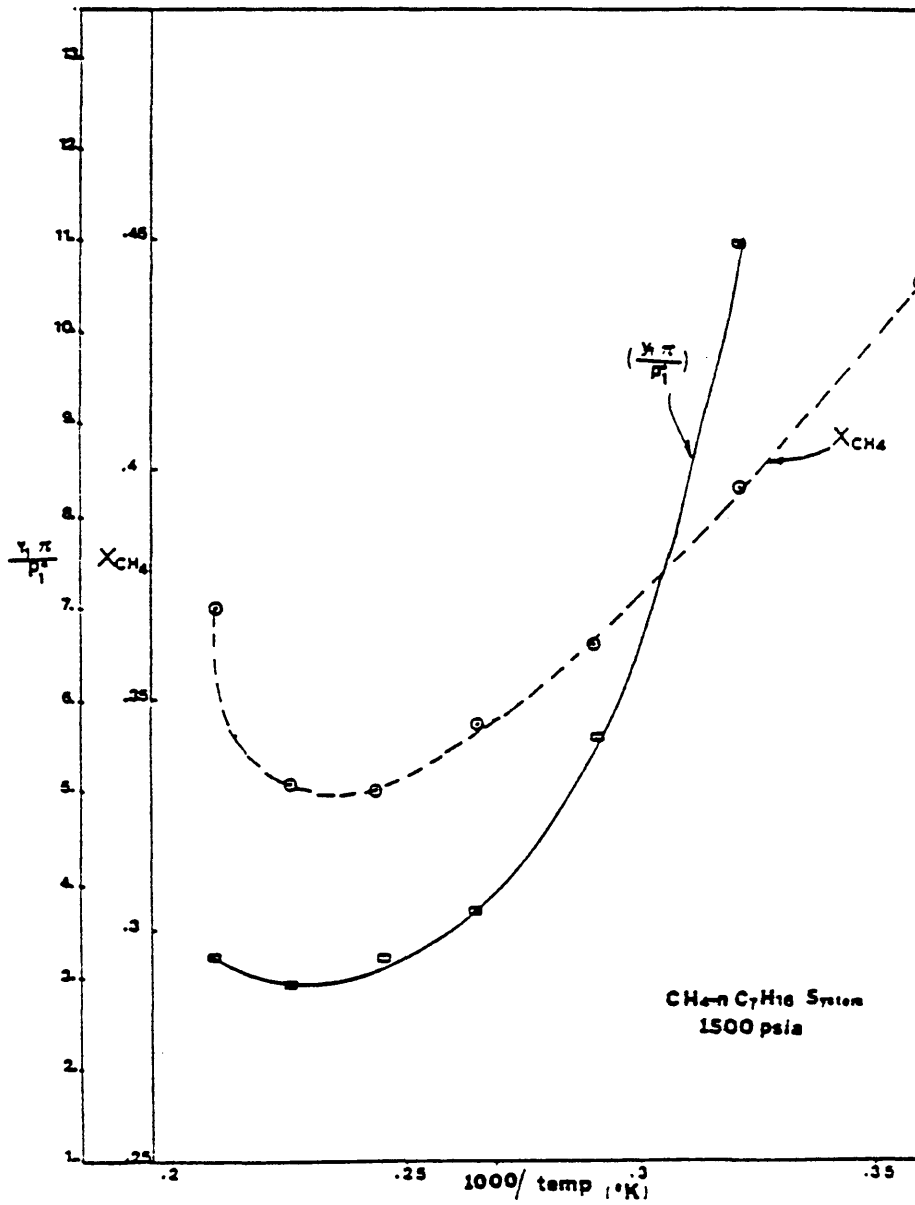
Those plots are shown in figure 34. A marked difference is observed between the slopes of the systems H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> and He-C<sub>2</sub>H<sub>6</sub>. In the same figure all systems that have slopes as steep as or

FIGURE No. 32



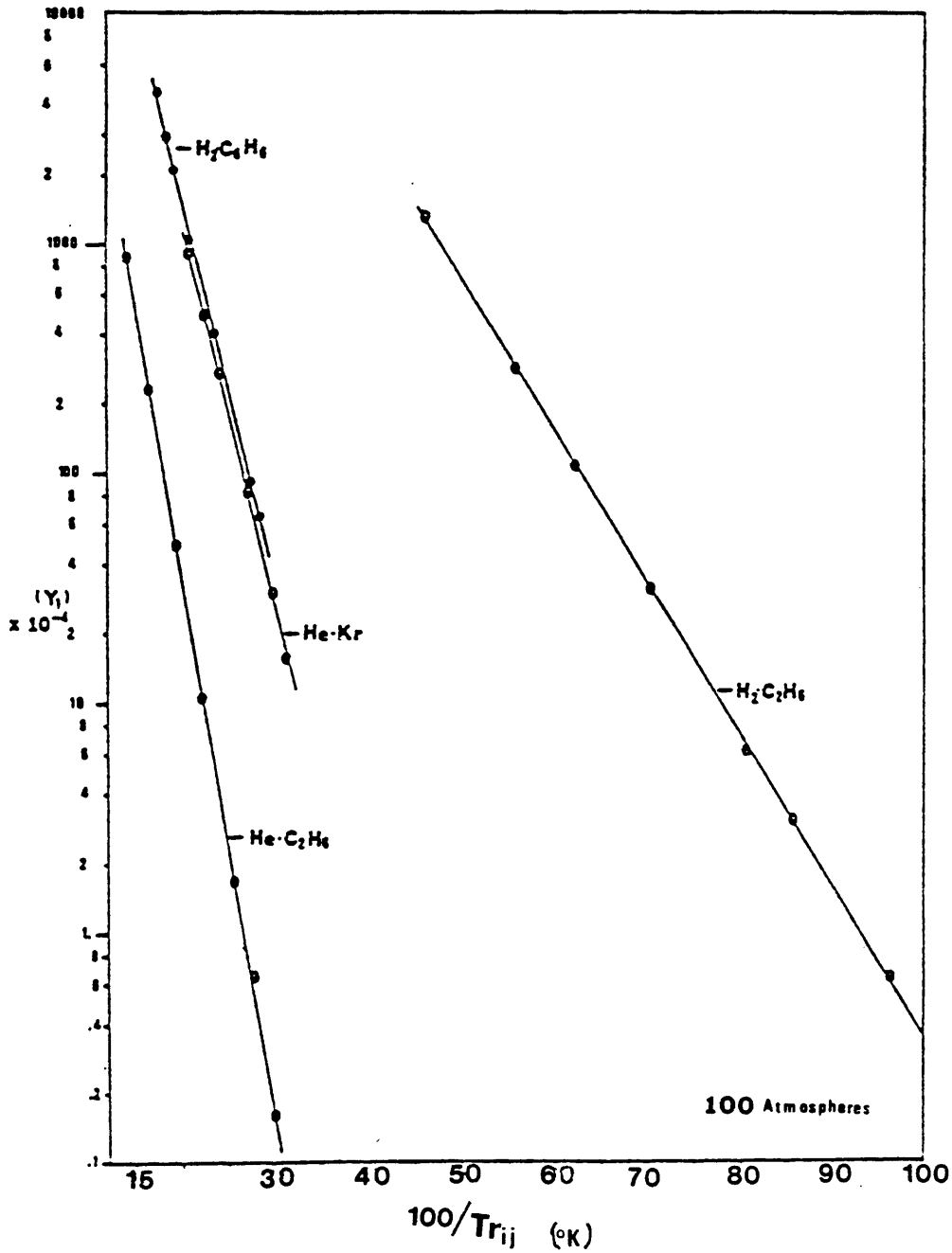
Plot of Mole Fraction of Heavy Component Versus Temperature in the He-C<sub>2</sub>H<sub>6</sub> and H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> System .

FIGURE No. 33



Enhancement Factor and Mole Fraction of light Component Versus Reciprocal Temperature in the CH<sub>4</sub>-nC<sub>7</sub>H<sub>16</sub> System

FIGURE No. 34

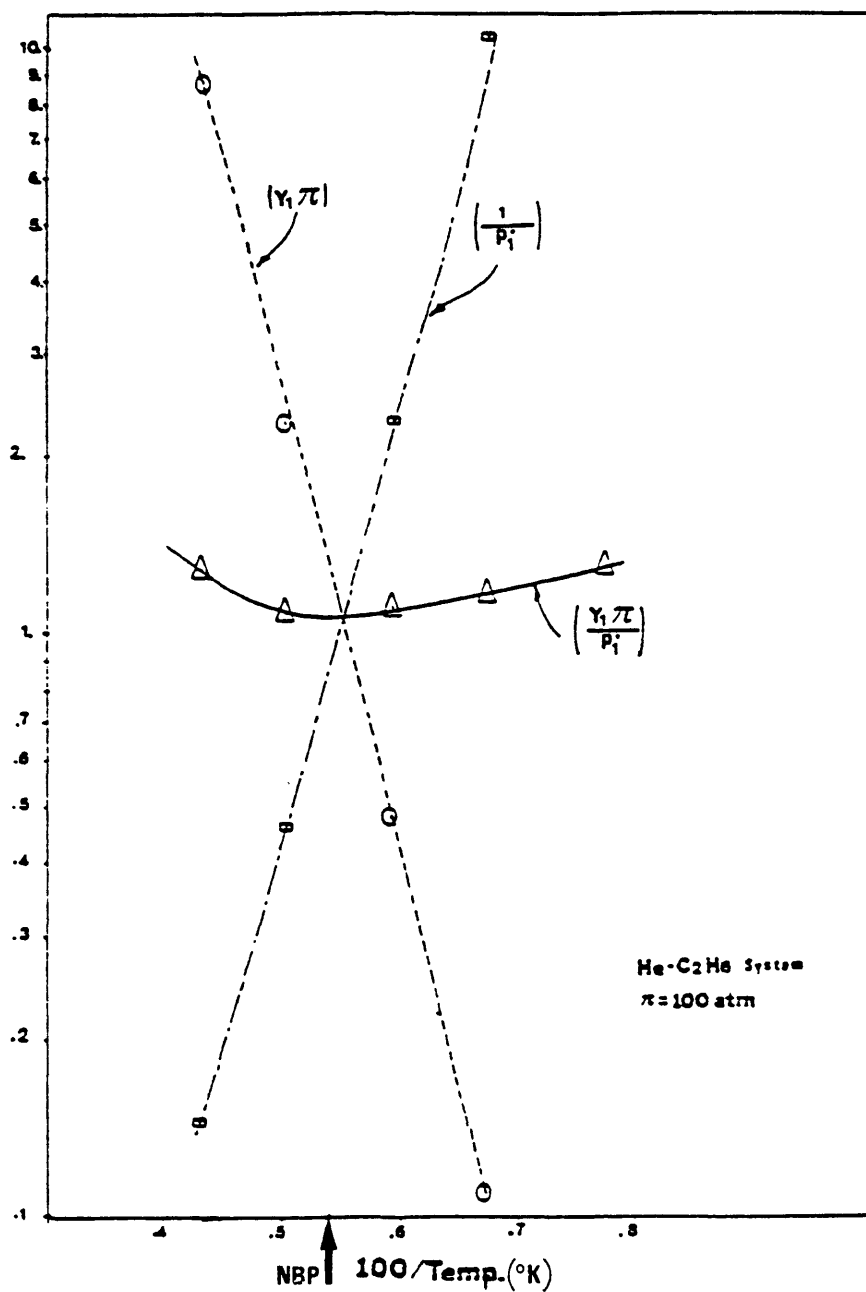


Plot of Mole Fraction of Heavy Component Versus Reciprocal Reduced Temperature Using Classical Critical Temperature for all Systems

steeper than that of the system  $H_2-C_6H_6$  have a pronounced minimum enhancement factor. In the  $H_2-C_2H_6$  system, which has a much less steep slope, the minimum enhancement factor is lacking. In order to clarify the plots of the enhancement factor against the reciprocal temperature, plots of reciprocal vapor pressure, and  $Y_1\pi$  versus reciprocal temperature were superimposed. These plots are shown in Figure 35, 36, 37, and 38, for the He- $C_2H_6$ , He-Kr,  $H_2-C_6H_6$  and  $H_2-C_2H_6$  systems, respectively. These plots show that the curves of the inverse of vapor pressure are intersected by the curves of near the normal boiling points for the first three systems. Figure 38 for the  $H_2-C_2H_6$  system presents only a moderate intersection; available data do not support an extension of the  $Y_1\pi$  line. While  $Y_1\pi/P_1^0$  should exhibit a minimum for He- $C_2H_6$ , He-Kr, and  $H_2-C_2H_6$ , a minimum is not clearly suggested for  $H_2-C_2H_6$ .

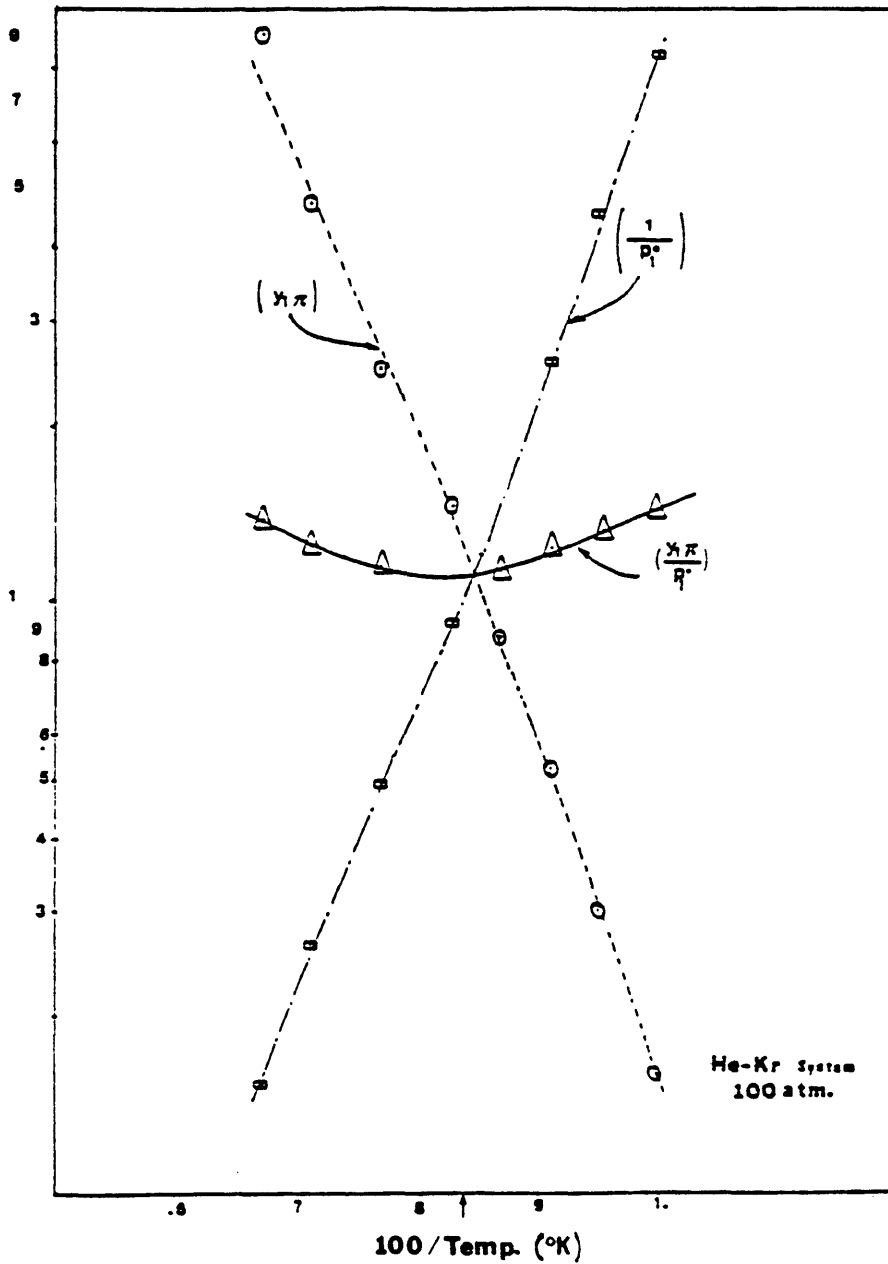
The higher solubility of  $H_2$  than He in  $C_2H_6$  shown in Figure 32 means that the mole fraction of  $C_2H_6$  ( $X_1$ ) is smaller in the  $H_2-C_2H_6$  system than in the He- $C_2H_6$  system. This result of this solubility difference was tested by means of equation (13), where the mole fraction of the heavy component should be considered.

FIGURE No. 35



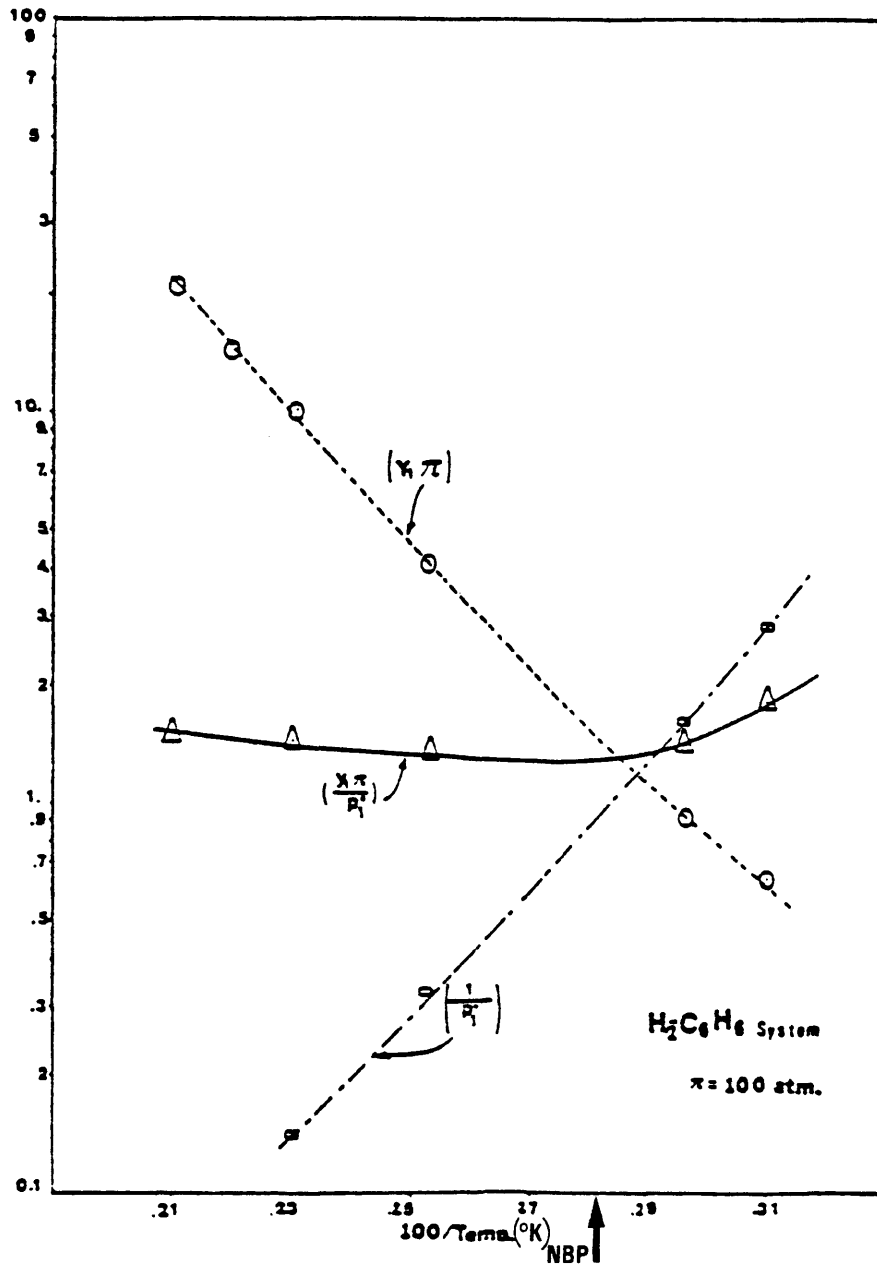
Plot of Enhancement Factor, Reciprocal Vapor Pressure, and  $Y_1\pi$  Versus Reciprocal Temperature of He-C<sub>2</sub>H<sub>6</sub> System

FIGURE No. 36



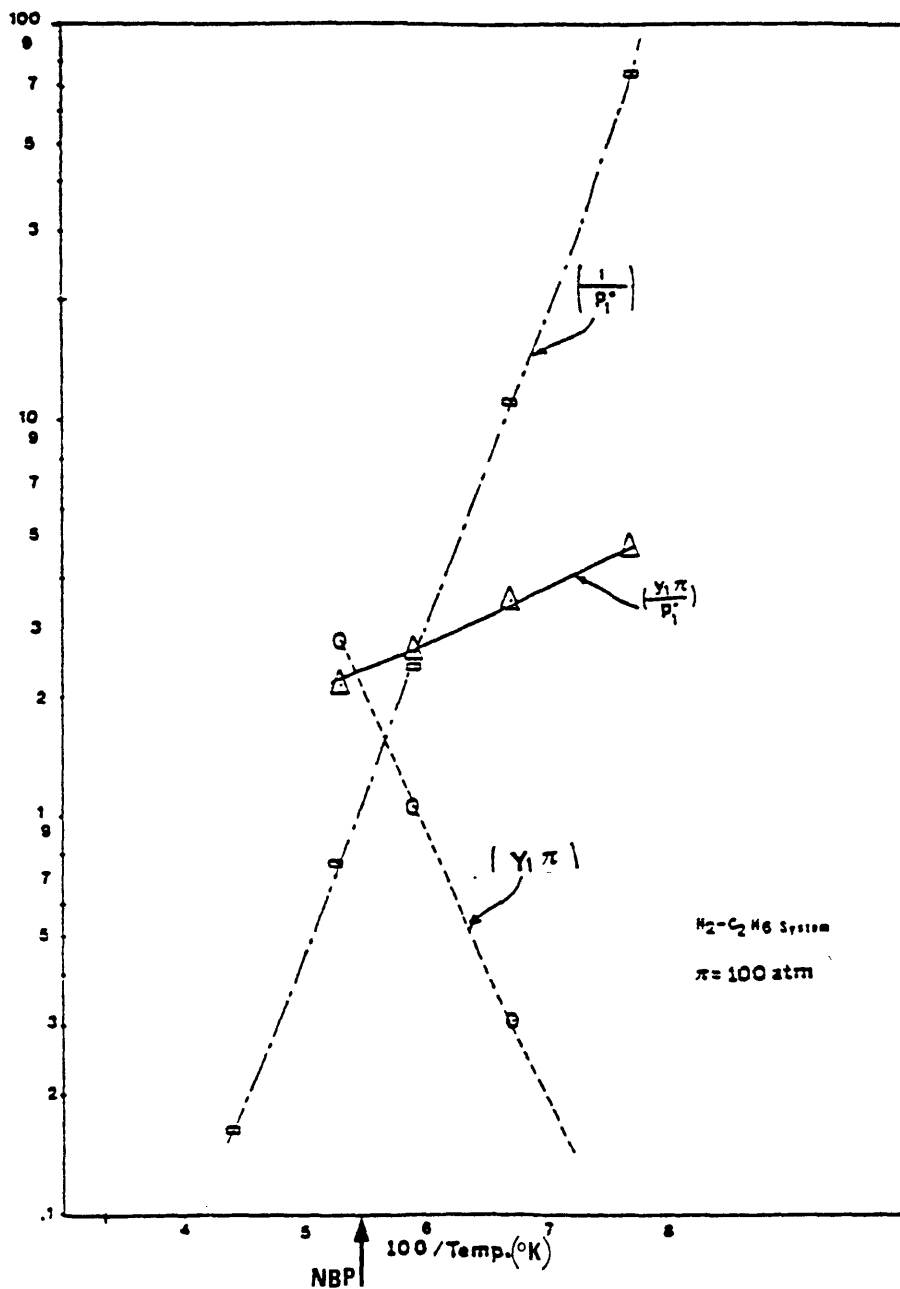
Plot of Enhancement Factor, Reciprocal Vapor Pressure,  
and  $Y_1\pi$  Versus Reciprocal Temperature of He-Kr System

FIGURE No. 37



Plot of Enhancement Factor, Reciprocal Vapor Pressure, and  $Y_1 \pi$  Versus Reciprocal Temperature of  $H_2-C_6H_6$  System

FIGURE No. 38



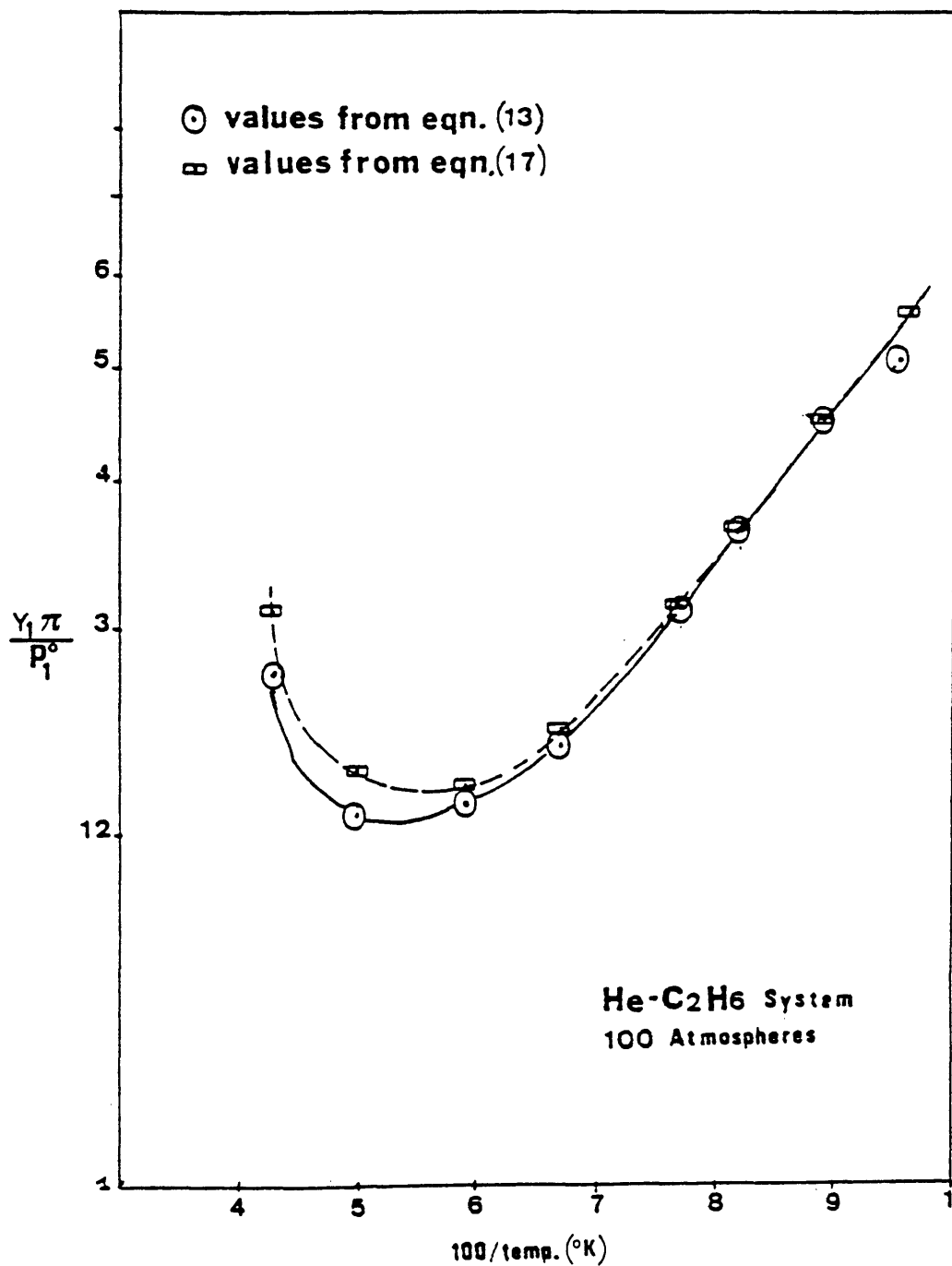
Plot of Enhancement Factor, Reciprocal Vapor Pressure, and  $Y_1 \pi$  Versus Reciprocal Temperature of  $H_2-C_2H_6$  System

The values of enhancement factor obtained from equation (13) were plotted against the reciprocal temperature in Figures 39 and 40. These plots show that the minimum enhancement factor still exists for the system He-C<sub>2</sub>H<sub>6</sub> and that for the system H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> the curve decreases monotonically as before.

Similar plots are shown for H<sub>2</sub>-C<sub>6</sub>H<sub>6</sub> and He-Kr system using Equation (13) in the Figure 41 and 42 respectively. The minimum for these systems still appears.

If the  $\gamma_1 \pi$  curve for H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> in Figure 37 were extrapolated without considering solubility a minimum could be predicted as shown in Figure 43.

FIGURE No. 39



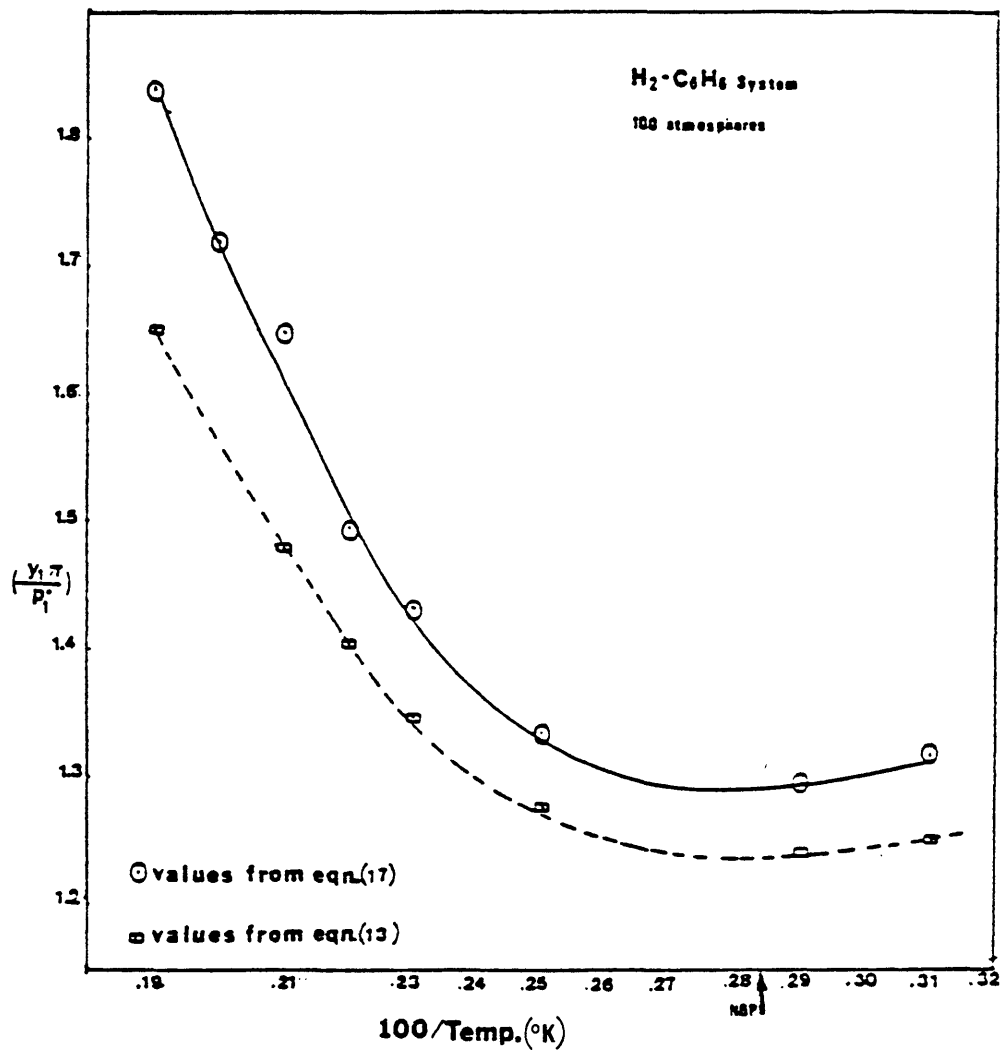
Enhancement Factor Versus Reciprocal Temperature Using Equations (13) and (17) for He-C<sub>2</sub>H<sub>6</sub> System

FIGURE No. 40



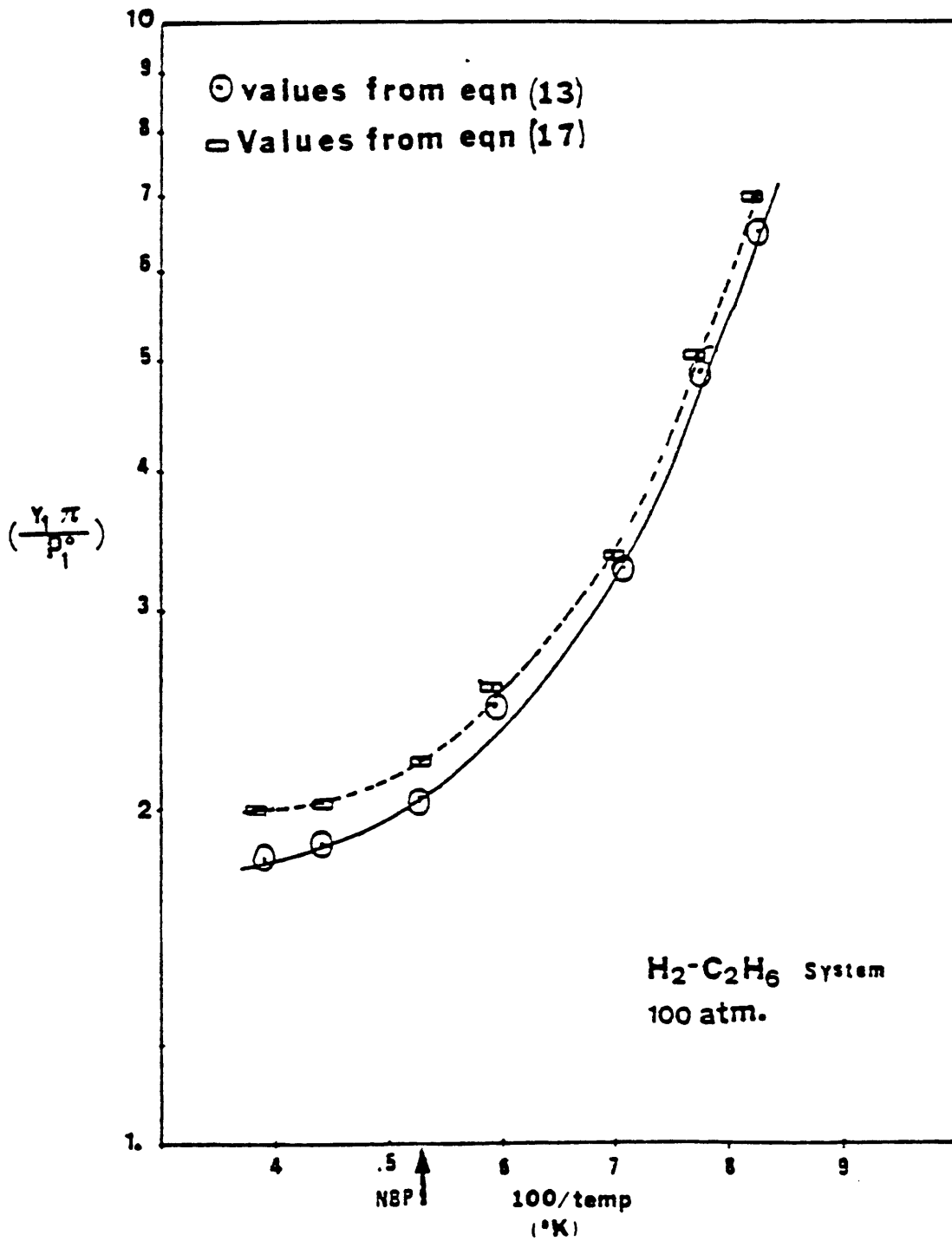
Enhancement Factor Versus Reciprocal Temperature Using Equations (13) and (17) for He-Kr system

FIGURE No. 41



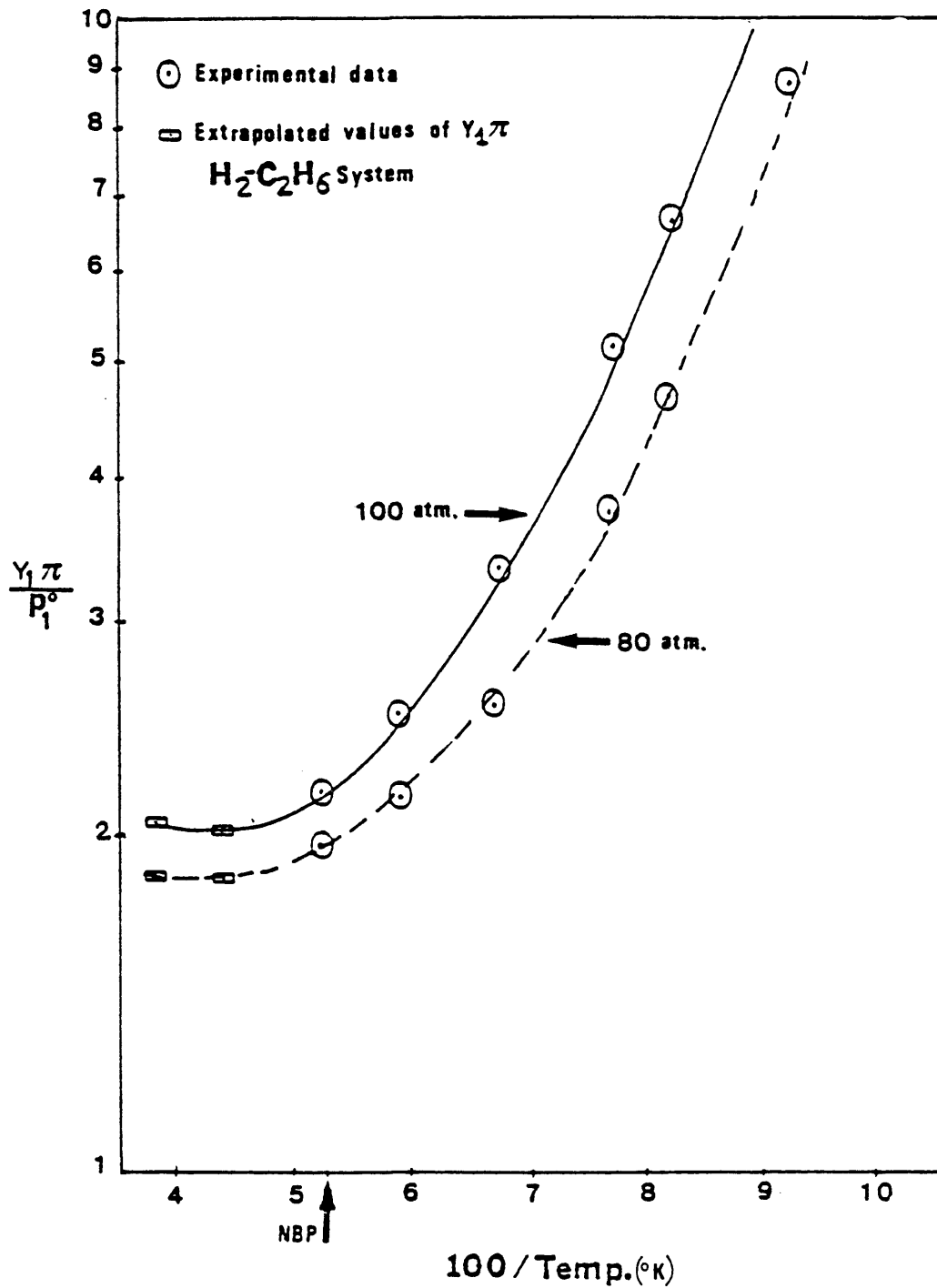
Enhancement Factor Versus Reciprocal Temperature Using Equations (13) and (17) for H<sub>2</sub>-C<sub>6</sub>H<sub>6</sub> system

FIGURE No. 42



Enhancement Factor Versus Reciprocal Temperature Using Equations (13) and (17) for  $H_2-C_2H_6$  System

FIGURE No. 43



Enhancement Factor Versus Reciprocal Temperature of  $\text{H}_2\text{-C}_2\text{H}_6$  System Extrapolating the Values of  $Y_1$  from Experimental Data

## CONCLUSION

In the systems for which liquid solubility is not a factor, the term  $2Y_1 B_{11} \pi / RT$  causes the minimum enhancement factor at reciprocal temperature. This minimum was evaluated for the systems He-C<sub>2</sub>H<sub>6</sub>, He-Kr, and H<sub>2</sub>-C<sub>6</sub>H<sub>6</sub>.

In the system H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub>, which does not have minimum enhancement factor, liquid solubility affects the enhancement factor, and the mole fraction of the heavy component in the liquid should be considered.

## RECOMMENDATION

Figure 34 shows that there is a close relationship between the slope of the graphs of the mole fraction versus the reciprocal reduced temperature of the systems studied. The system that exhibits a minimum enhancement factor showed closely related gradients but the system that does not show a minimum enhancement factor shows an entirely different slope. Hence it is recommended that the future investigations should be directed towards the exact determination of slope which a minimum appears.

NOMENCLATURE

- $a$  = core radius  
 $a^*$  = reduced core size  
 $B$  = second virial coefficient  
 $b$  = coefficients for series representation of  $F_i$   
 $C$  = third virial coefficient  
 $C_1^0$  = constant given by classical critical temperature equation (28) and equals 21.8 °K  
 $C_2^0$  = constant given by classical critical volume equation (29) and equals -9.91 °K  
 $d$  = empirical parameter characterizing polarizability  
 $f_i^0$  = standard-state fugacity of component "i"  
 $f_i^v$  = fugacity of the component "i" in vapor phase  
 $f_i^L$  = fugacity of the component "i" in liquid phase  
 $f_i^s$  = fugacity of the component "i" in solid phase  
 $F$  = function of the Kihara core model  
 $k$  = Boltzman's constant  
 $m$  = molecular mass

$M_o, S_o, V_o,$  = parameter of Kihara model

$N_a$  = Avogadro's number

$n_i$  = moles number (component "i")

$n_j$  = moles number (component "j")

$p_i^o$  = vapor pressure of component "i"

$R$  = gas constant

$r_{ij}$  = distance between molecules "i" and "j"

$T$  = temperature of system

$T_p$  = triple point temperature

$T_c$  = critical temperature

$T_r$  = reduced temperature

$T_c^o$  = classical critical temperature

$T^*$  =  $kT/\epsilon$

$T_o$  = temperature of reference of Goodwin correlation = 217.8 °K

$U$  = potential energy

$U_o$  = maximum (negative) potential energy

$V_i$  = volume of component "i"

$V_c$  = critical volume

$V_c^o$  = classical critical volume

$X_i$  = molar fraction of component "i" in liquid phase

$Y_i$  = molar fraction of component "i" in vapor phase

$Z$  =  $U_o/kT$

Greek Letters

$\gamma_i$  = activity coefficient

$\pi$  = total pressure

$\phi_i^o$  = fugacity coefficient of component "i" in solid or liquid phase

$\phi_i$  = fugacity coefficient of component "i" in the vapor phase mixture

$\epsilon$  = enhancement factor

$\rho$  = density

$\rho_o$  = the shortest distance between molecular core at minimum potential energy

$\rho$  = the shortest distance between molecular core

$\sigma$  = separation of molecular center of zero potential energy

$\omega$  = acentric factor

Superscripts

o = pure vapor pressure

l = liquid phase

s = solid phase

v = vapor phase

Subscripts

- i = component 1
- j = component 2
- a = for Avogadro's number
- c = to indicate critical condition
- r = to indicate a reduced condition
- s = summation index integer, also dummy variable for Kihara coefficients

## VARIABLES DEFINITION IN THE COMPUTER PROGRAM

ANAV	Avogadro's numbers
AKB	Boltzman's constant
AMM1	Molecular weight component 1
AMM2	Molecular weight component 2
A1,A2,A3,A4,A5,	Parameter of Goodwin
B11	Second virial component 1
B22	Second virial coefficients component 1
B12	Second virial cross coefficients
CEN(I,L)	Enhancement factor experimental
C111	Third virial coefficients
C222	Third virial coefficients component 2
C122	Third virial cross coefficients
C112	Third virial cross coefficients
DDE1	Density of ethane
DIS1	Shortest distance between molecular cores at energy minimum (component 1)
DIS2	Shortest distance between molecular cores at energy minimum (component 2)
DIS	Shortest distance average between components 1 and 2
DED012	Empirical parameter characterizing polariza- bility size and shape of a molecule
D1,D2,D3,D4	Parameters of Goodwin
ENH(I,L)	Enhancement factor calculated from equation (17)
ENX	Enhancement factor calculated from equation (13)

F1	Kihara coefficient
F2	Kihara coefficient
F3	Kihara coefficient
H1,H2,H3	Parameter of Goodwin
M	Iteration to calculate the coefficients of Kihara
NT	Number of isotherms into the system
PKM1	Parameter of Kihara core component 1
PKM2	Parameter of Kihara core component 2
PREVM	Vapor Pressure
PRECTM	Pressure critical of ethane
PRETFM	Pressure of triple point of ethane
PT	Total pressure
PO	Value of conversion of bar to atmosphere
SUR1	Surface parameter of Kihara component 1
SUR2	Surface parameter of Kihara component 2
TECE12	Critical temperature of mixture
TRR	Reduced temperature of mixture
TEC2	Effective critical temperature component 2
TECE02	Critical temperature of component 2
TERE	Reduced temperature
TEMPM	Temperature of the systems
TETPM	Temperature of triple point
TECE1	Temperature critical

TETOE	Temperature of Reference given by Goodwin
UNER1	Maximum potential energy divided by Boltzman's constant component 1
UNER2	Maximum potential energy divided by Boltzman's constant component 2
UNER12	Potential energy of mixture
UKV	Prausnitz parameter
VOLU1	Volume parameter of Kihara component 1
VOLU2	Volume parameter of Kihara component 2
VLC2	Classical critical volume component 2
VLC12	Effective critical volume of mixture
VOLM	Volume of liquid
XC1	Constant given to calculate the effective critical temperature
XC2	Constant given to calculate the effective critical volume
XL1	Composition of liquid phase component 1
YV1	Composition of vapor phase component 1
YV2	Composition of vapor phase component 2
ZUF	Potential energy divided by temperature

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A P P E N D I X    A  
C O M P U T E R   L I S T I N G

```

C
C ***** MAIN PROGRAM *****
C
C PHASE.FOR
C
C PROGRAM PHASE1
C
C PROGRAM TO CALCULATE THE ENHANCEMENT FACTOR USING THE
C EXACT EQUATION OF GOODWIN,RODER AND STARTY.
C
C SELECT THE BINARY SYSTEM TO BE USED
C
C NSYS=1 FOR HE-C2H6
C NSYS=2 FOR HE-KR
C NSYS=3 FOR H2-C6H6
C NSYS=4 FOR H2-C2H6
C
C DIMENSION TERE(9),VOLM(9),ENH(9,6),PT(9,6),CEN(9,6),
1 PREVM(9),DIFF(9,6),ENX(9,6),XL1(9,6),DXFF(9,6)
C DOUBLE PRECISION TET1,TET2,TET3,PET1,PET2,PET3,SET1,
1 SET2,SET3
C COMMON /BLO/ P1(9,6),P2(9,6),P3(9,6),P4(9,6)
C COMMON /MAIN/ TEMPM(9),NT,NV,B(9),B11(9),B22(9),B12(9),
1 C111(9),C112(9),C122(9),C222(9),YVE(9,6),YV1(9,6),
2 YV2(9,6),TECE1,PRECTM,PENTPM(9),UKV,
3 ANAV,DIS1,DIS2,PKM1,PKM2,SUR1,SUR2,VOLU1,VOLU2,
4 UNER1,UNER2,DIS,PKM,SUR,VOLU,UNER,TECE02,AMM1,
5 AMM2,XC1,XC2,VLC1,VLC2,EX,Y1(9,6),Y2(9,6),
6 Y3(9,6),Y4(9,6),X1(9,6),X2(9,6),X3(9,6),
7 X4(9,6),EF1(9,6),EF2(9,6),EF3(9,6),EF4(9,6),
8 NSYS,DEDD12
C DATA EXO,PO,TETPM,TECE1,TETOE,PRECTM,ODE1,PRETPM/
1 1.3,.9869,90.348,305.53,217.8,48.71,.00674,
2 1.1308E-05/
C DATA A1,A2,A3,A4,A5,A6,D1,D2,D3,D4,H1,H2,H3/
1 -11.38996,18.84522,-7.63541,5.42844,-1.36232,
2 .76924,.552671,-1.106244,-.59294,-.041944,.244423,
3 .93253,.53488/
C
C TYPE 1
1 FORMAT('INPUT DATA:SYSTEM TYPE='$)
C ACCEPT 2,NSYS
2 FORMAT(I)
C
C R=82.05
C NT=9
C NV=6
C IF(NSYS.EQ.1)GO TO 11
C IF(NSYS.EQ.2)GO TO 22
C IF(NSYS.EQ.3)GO TO 33
C IF(NSYS.EQ.4)GO TO 11
C

```

```

11  CONTINUE
    IF(NSYS.EQ.4)GO TO 44
C   READ THE DATA FOR THE HE-C2H6 SYSTEM
    READ(11,41)DIS1,DIS2,PKM1,PKM2,SUR1,SUR2
    READ(11,41)VOLU1,VOLU2,UNER1,UNER2,AMM1,AMM2
    READ(11,42)VLC1,VLC2,TECE02,UKY,DEDO12,EX
    READ(11,43)(TEMPM(I),I=1,NT)
    READ(11,43)(VOLM(I),I=1,NT)
    READ(11,43)(C222(I),I=1,NT)
    DIS=DIS2
    PKM=PKM2
    SUR=SUR2
    VOLU=VOLU2
    UNER=UNER2
C   CALCULATE THE SECOND VIRIAL COEFFICIENT OF HELIUM
C
C   CALL NAPO
C
C   DO 29 I=1,NT
        B22(I)=B(I)
29  CONTINUE
C
C.....NOW START THE CALCULATION APLAIED THE EQN.#2,#4(A) AND
C.....#4(B) OF GOODWIN CORRELATION
C
    DO 30 I=1,NT
        TERE(I)=TEMPM(I)/TECE1
        W1=(1.-TETPM/TEMPM(I))/(1.-TETPM/TECE1)
        X0=(TEMPM(I)-TETPM)/(TECE1-TETPM)
        U1=X0
        U2=U1*U1
        U3=U2*U1
        XB=A1+A2*W1+A3*U1+A4*U2+A5*U3+A6*U1*((1.-U1)**EXD)
        XBA=EXP(XB)
        PREVMI(I)=XBA*PO
C.....CALCULATE THE COEFF. B11 FOR ETHANE FROM EQN. 4(A)
        WA1=TERE(I)
        WA2=WA1**2
        WA4=WA1**4.5
        BV1=D1+D2/WA1+D3/WA2+D4/WA4
        B11(I)=BV1/DDE1
C.....CALCULATE THE COEFF. C111 FOR ETHANE FROM EQN. 4(B)
C
        Z1=WA1
        Z3=Z1**3
        Z5=Z1**5
        CE1=(H1/Z1+H2/Z3+H3/Z5)*(1.-TETDE/TEMPM(I))
        C111(I)=CE1/DDE1
30  CONTINUE
C.....NOW CALCULATE THE COEFF.B12 WITH SUBROUTINE

```

```

C.....
      CALL PIPA
C.....
C.....NOW CALCULATE THE COEFF. C12
C
      CALL LIRA
C
      GO TO 77
44      CONTINUE
C      READ THE DATA FOR H2-C2H6 SYSTEM
C
      READ(14,41)DIS1,DIS2,PKM1,PKM2,SUR1,SUR2
      READ(14,41)VOLU1,VOLU2,UNER1,UNER2,AMM1,AMM2
      READ(14,42)VLC1,VLC2,TECE02,UKV,DEDO12,EX
      READ(14,43)(TEMPM(I),I=1,NT)
      READ(14,43)(VOLM(I),I=1,NT)
      READ(14,43)(C222(I),I=1,NT)
      DIS=DIS2
      PKM=PKM2
      SUR=SUR2
      VOLU=VOLU2
      UNER=UNER2
C
C
      CALL NAPO
      DO 31 I=1,NT
          B22(I)=B(I)
31      CONTINUE
C.....NOW START THE CALCULATION APLAIED THE EQN.#2,#4(A) AND
C.....#4(B) OF GOODWIN CORRELATION
C
      DO 32 I=1,NT
          TERE(I)=TEMPM(I)/TECE1
          W1=(1.-TETPM/TEMPM(I))/(1.-TETPM/TECE1)
          X0=(TEMPM(I)-TETPM)/(TECE1-TETPM)
          U1=X0
          U2=U1*U1
          U3=U2*U1
          XB=A1+A2*W1+A3*U1+A4*U2+A5*U3+A6*U1*((1.-U1)**EX0)
          XBA=EXP(XB)
          PREVH(I)=XBA*PO
C.....CALCULATE THE COEFF. B11 FOR ETHANE FROM EQN. 4(A)
          WA1=TERE(I)
          WA2=WA1**2
          WA4=WA1**4.5
          BV1=D1+D2/WA1+D3/WA2+D4/WA4
          B11(I)=BV1/DDE1
C.....CALCULATE THE COEFF. C111 FOR EHANE FROM EQN. 4(B)
C
          Z1=WA1
          Z3=Z1**3

```

```

          Z5=Z1**5
          CE1=(H1/Z1+H2/Z3+H3/Z5)*(1.-TETDE/TEMPM(I))
          C111(I)=CE1/DDE1
32      CONTINUE
C.....NOW CALCULATE THE COEFF. B12 WITH SUBROUTINE
      CALL PIPA
C
C
C      NOW CALCULATE THE THIRD VIRIAL CROSS COEFFICIENT C112
C      AND C122
C
C      CALL LIRA
C
C      GO TO 77
C
22     CONTINUE
C
C      READ THE DATA FOR HE-KR SYSTEM
C
      READ(12,41)DIS1,DIS2,PKM1,PKM2,SUR1,SUR2
      READ(12,41)VOLU1,VOLU2,UNER1,UNER2,AMM1,AMM2
      READ(12,41)VLC1,VLC2,TECE02,UKV,DEDO12,EX
      READ(12,54)TETPM,TECE1,PRECTM,DDE1,PRETPM
      READ(12,43)(TEMPM(I),I=1,NT)
      READ(12,43)(VOLM(I),I=1,NT)
      READ(12,43)(PREVM(I),I=1,NT)
      READ(12,43)(C111(I),I=1,NT)
      READ(12,43)(C222(I),I=1,NT)
      DIS=DIS2
      PKM=PKM2
      SUR=SUR2
      VOLU=VOLU2
      UNER=UNER2
C      CALCULATE THE SECOND VIRIAL COEFFICIENT OF HELIUM
      CALL NAPO
      DO 34 I=1,NT
          B22(I)=B(I)
34     CONTINUE
C
C
      DIS=DIS1
      PKM=PKM1
      SUR=SUR1
      VOLU=VOLU1
      UNER=UNER1
C      CALCULATE THE SECOND VIRIAL COEFFIECIENTS OF KR
C
      CALL NAPO
      DO 35 I=1,NT
          B11(I)=B(I)
35     CONTINUE

```

```

C      NOW CALCULATE THE COEFF. B12
C
C      CALL PIPA
C
C      NOW CALCULATE THE COEFF. C122 AND C112
C
C      CALL LIRA
C      GO TO 77
33     CONTINUE
C
C
C      READ THE DAT FOR H2-C6H6 SYSTEM
C
C      READ(13,41)DIS1,DIS2,PKM1,PKM2,SUR1,SUR2
C      READ(13,41)VCLU1,VOLU2,UNER1,UNER2,AMM1,AMM2
C      READ(13,41)VLC1,VLC2,TECE02,UKV,DEDO12,EX
C      READ(13,43)TECE1,TEB01,PRECTM
C      READ(13,43)(TEMPM(I),I=1,NT)
C      READ(13,43)(C111(I),I=1,NT)
C      READ(13,43)(C222(I),I=1,NT)
C
C      DIS=DIS1
C      PKM=PKM1
C      SUR=SUR1
C      VOLU=VOLU1
C      UNER=UNER1
C      NOW CALCULATE THE SECOND VIRIAL COEFFICIENTS FOR
C      BENZENE.
C      CALL NAPO
C      DO 36 I=1,NT
C          B11(I)=B(I)
36     CONTINUE
C
C      DIS=DIS2
C      PKM=PKM2
C      SUR=SUR2
C      VOLU=VOLU2
C      UNER=UNER2
C      NOW CALCULATE THE SECOND VIRIAL COEFFICIENTS FOR
C      HYDROGEN.
C      CALL NAPO
C      DO 37 I=1,NT
C          B22(I)=B(I)
37     CONTINUE
C
C      CALCULATE THE ACENTRIC FACTOR
C
C      TT1=TEB01/TECE1
C      TT2=-ALOG(PRECTM)-5.92714+(6.096480/TT1)+1.28862*(ALOG(TT1))
C      TT3=0.169347*(TT1**6)
C      TT4=TT2-TT3

```

```

TT5=15.2518-15.6875/TT1-13.4721*(ALOG(TT1))+0.43577*TT1**6
ACFW=TT4/TT5

```

```

C
C
C
C

```

```

CALCULATE THE VAPOR PRESSURE FOR THE BENZENE

```

```

DO 38 K=1,NT
  TERE(K)=TEMPM(K)/TECE1
  W1=ALOG(TERE(K))
  W2=TERE(K)**6
  TIPO=5.92714-6.09648/TERE(K)-1.28862*W1+0.169347*W2
  TIP1=15.2518-15.6875/TERE(K)-13.4721*W1+0.43577*W2
  TIP2=TIP0+TIP1*ACFW
  PREVM(K)=EXP(TIP2)*PRECTM

```

```

C
C

```

```

CALCULATE THE VOLUME

```

```

T1=TERE(K)
T2=T1**2.
T3=T1**3.
T4=T1**4.
TAO=0.29607-0.09045*T1-0.04842*T2
VSC=R*TECE1*(0.2920-0.0967*ACFW)/PRECTM
VRO=0.33593-0.33593*T1+1.51941*T2-2.02512*T3+1.1422*T4
VOLM(K)=VRO*(1.-ACFW*TAO)*VSC
CONTINUE

```

```

38

```

```

C
C
C
C

```

```

NOW CALCULATE THE COEFF. B12

```

```

CALL PIPA

```

```

C
C
C

```

```

NOW CALCULATE THE COEFF. C112 AND C122

```

```

CALL LIRA

```

```

C
C
C

```

```

GO TO 77

```

```

77

```

```

CONTINUE
DO 60 I=1,NT
  IF(NSYS.EQ.3)NV=4
  DO 70 L=1,NV
    IF(NSYS.EQ.1)GO TO 40
    IF(NSYS.EQ.2)GO TO 141
    IF(NSYS.EQ.3)GO TO 142
    IF(NSYS.EQ.4)GO TO 143

```

```

40

```

```

PT(I,L)=P1(I,L)
XL1(I,L)=X1(I,L)
CEN(I,L)=EF1(I,L)
GO TO 64

```

```

141

```

```

PT(I,L)=P2(I,L)

```

```

XL1(I,L)=X2(I,L)
CEN(I,L)=EF2(I,L)
GO TO 64
142 PT(I,L)=P3(I,L)
XL1(I,L)=X3(I,L)
CEN(I,L)=YV1(I,L)*PT(I,L)/PREVM(I)
GO TO 64
143 PT(I,L)=P4(I,L)
XL1(I,L)=X4(I,L)
CEN(I,L)=EF4(I,L)
64 CONTINUE
RA1=YV1(I,L)
E1= VOLM(I)*(PT(I,L)-PREVM(I))/(R*TEMPM(I))
E2=B11(I)*PREVM(I)/(R*TEMPM(I))
E3=(2.*RA1-YV1(I,L)**2)*B11(I)*PT(I,L)/(R*TEMPM(I))
E4=(C111(I)-B11(I)**2)*PREVM(I)**2/(((R*TEMPM(I))**2)*2.)
EE2=E2+E4
E5=(B22(I)-B12(I)*2.)*YV2(I,L)**2*PT(I,L)/(R*TEMPM(I))
E6=PT(I,L)**2/(((R*TEMPM(I))**2)*2.)
EA1=3.*YV2(I,L)**2*C122(I)
EA2=6.*YV1(I,L)*YV2(I,L)*C112(I)
EA3=3.*YV1(I,L)**2*C111(I)
EA4=YV2(I,L)**3*(2.*C222(I)+4.*B12(I)*B22(I))
EA5=YV1(I,L)*YV2(I,L)**2*(6.*C122(I)+4.*B11(I)*B22(I)+
1 8.0*B12(I)**2)
EA6=YV1(I,L)**2*YV2(I,L)*(12.*B11(I)*B12(I)+6.*C112(I))
EA7=YV1(I,L)**3*(4.*B11(I)**2+2.*C111(I))
EA8=YV2(I,L)**4*(3.*B22(I)**2)
EA9=YV1(I,L)*YV2(I,L)**3*(12.*B12(I)*B22(I))
EA10=YV1(I,L)**2*YV2(I,L)**2*(6.*B11(I)*B22(I)+12.*B12(I)**2)
EA11=YV1(I,L)**3*YV2(I,L)*(12.*B12(I)*B11(I))
EA12=YV1(I,L)**4*(3.*B11(I)**2)
AF=-EA1-EA2-EA3+EA4+EA5+EA6+EA7-EA8-EA9-EA10-EA11-EA12
AF1=AF*E6
EE3=-E3+E5+AF1
AF2=E1+E2-E3+E4+E5+AF1
ENH(I,L)=EXP(AF2)
AF8=AF2+ALOG(XL1(I,L))
ENX(I,L)=EXP(AF8)
DXFF(I,L)=(ABS(ENH(I,L)-CEN(I,L))/CEN(I,L))*100.0
DIFF(I,L)=(ABS(ENX(I,L)-CEN(I,L))/CEN(I,L))*100.0
C
70 CONTINUE
60 CONTINUE
WRITE(10,113)
113 FORMAT(8X,"TEMP",6X,"VOL",6X,"VAPRES",5X,"MDLFYV1",3X,
1 "SYSPRES",4X,"ENH+X",5X,"ENH-X",3X,"EXPENH",2X,
2 "PERDEV",3X,"REF"/6X,95("=)//)
114 FORMAT(4X,2F9.2,2E12.2,5F9.2/5(34X,E12.2,5F9.2//)
WRITE(1,115)(TEMPM(I),B11(I),B22(I),B12(I),C111(I),
1 C222(I),C122(I),C112(I),I=1,9)

```

```
115  FORMAT(F10.2,2X,7E11.2/)
      DO 45 I=1,NT
      IF(NSYS.EQ.3)NV=4
      WRITE(10,114)(TEMPM(I),VOLM(I),PREVM(I),(YVI(I,L),PT(I,L),
1  ENH(I,L),ENX(I,L),CEN(I,L),DIFF(I,L),L=1,NV))
45   CONTINUE
41   FORMAT(6F)
42   FORMAT(5F,E)
43   FORMAT(3F)
54   FORMAT(5F)
      END
```

## BLOCK DATA

```

COMMON /BLO/ P1(9,6),P2(9,6),P3(9,6),P4(9,6)
COMMON /MAIN/ TEMPM(9),NT,NV,B(9),B11(9),B22(9),B12(9),
1  C111(9),C112(9),C122(9),C222(9),YVE(9,6),YV1(9,6),
2  YV2(9,6),TECE1,PRECTM,PEMTPM(9),UKV,
3  ANAV,DIS1,DIS2,PKM1,PKM2,SUR1,SUR2,VOLU1,VOLU2,
4  UNER1,UNER2,DIS,PKM,SUR,VOLU,UNER,TECE02,AMM1,
5  AMM2,XC1,XC2,VLC1,VLC2,EX,Y1(9,6),Y2(9,6),
6  Y3(9,6),Y4(9,6),X1(9,6),X2(9,6),X3(9,6),
7  X4(9,6),EF1(9,6),EF2(9,6),EF3(9,6),EF4(9,6),
8  NSYS,DEDO12

```

```

READ THE TOTAL PRESSURE,MOLAR FRACTION OF ETHANE
IN THE VAPOR AND LIQUID PHASE, EXPERIMENTAL ENHEN
HANCENT FACTOR.

```

```

DATA P1(1,1),P1(1,2),P1(1,3),P1(1,4)/17.4,26.2,40.6,60.6/,
1  P1(1,5),P1(1,6),P1(2,1),P1(2,2)/84.7,117.0,8.8,24.8/,
2  P1(2,3),P1(2,4),P1(2,5),P1(2,6)/49.2,78.0,102.7,139.9/,
3  P1(3,1),P1(3,2),P1(3,3),P1(3,4)/14.9,29.9,49.9,69.9/,
4  P1(3,5),P1(3,6),P1(4,1),P1(4,2)/89.1,119.1,26.2,46.95/,
5  P1(4,3),P1(4,4),P1(4,5),P1(4,6)/70.6,80.9,98.6,118.2/,
6  P1(5,1),P1(5,2),P1(5,3),P1(5,4)/4.5,22.49,44.95,71.3/,
7  P1(5,5),P1(5,6),P1(6,1),P1(6,2)/98.8,130.4,10.72,25.99/
DATA P1(6,3),P1(6,4),P1(6,5),P1(6,6)/45.08,71.2,100.1,129.0/,
1  P1(7,1),P1(7,2),P1(7,3),P1(7,4)/5.82,14.4,25.72,45.38/,
2  P1(7,5),P1(7,6),P1(8,1),P1(8,2)/99.6,128.1,3.98,13.0/,
3  P1(8,3),P1(8,4),P1(8,5),P1(8,6)/26.0,43.45,68.8,128.0/,
4  P1(9,1),P1(9,2),P1(9,3),P1(9,4)/4.1,10.35,15.32,23.25/,
5  P1(9,5),P1(9,6)/46.2,46.5/
DATA Y1(1,1),Y1(1,2),Y1(1,3)/445000.0,305000.0,199000.0/,
1  Y1(1,4),Y1(1,5),Y1(1,6)/137000.0,100500.0,73800.0/,
2  Y1(2,1),Y1(2,2),Y1(2,3)/251000.0,92100.0,48700.0/,
3  Y1(2,4),Y1(2,5),Y1(2,6)/30500.0,23900.0,17800.0/,
4  Y1(3,1),Y1(3,2),Y1(3,3)/28700.0,14600.0,9050.0/,
5  Y1(3,4),Y1(3,5),Y1(3,6)/6640.0,5350.0,4140.0/,
6  Y1(4,1),Y1(4,2),Y1(4,3)/3682.0,2133.0,1493.0/,
7  Y1(4,4),Y1(4,5),Y1(4,6)/1283.0,1078.0,865.3/,
8  Y1(5,1),Y1(5,2),Y1(5,3)/2846.0,600.0,323.1/,
9  Y1(5,4),Y1(5,5),Y1(5,6)/215.2,173.9,141.3/
DATA Y1(6,1),Y1(6,2),Y1(6,3)/439.1,200.4,121.7/,
1  Y1(6,4),Y1(6,5),Y1(6,6)/83.48,65.21,55.22/,
2  Y1(7,1),Y1(7,2),Y1(7,3)/176.1,79.57,47.83/,
3  Y1(7,4),Y1(7,5),Y1(7,6)/29.35,16.57,14.57/,
4  Y1(8,1),Y1(8,2),Y1(8,3)/43.26,14.78,8.145/,
5  Y1(8,4),Y1(8,5),Y1(8,6)/5.445,3.877,2.71/,
6  Y1(9,1),Y1(9,2),Y1(9,3)/9.495,4.189,2.994/,
7  Y1(9,4),Y1(9,5),Y1(9,6)/2.049,1.181,1.149/

```

```

DATA X1(1,1),X1(1,2),X1(1,3)/.974,.981,.9865/,
1  X1(1,4),X1(1,5),X1(1,6)/.9915,.996,.997/,

```

```

2  X1(2,1),X1(2,2),X1(2,3)/.983,.987,.99/,
3  X1(2,4),X1(2,5),X1(2,6)/.994,.997,.999/,
4  X1(3,1),X1(3,2),X1(3,3)/.993,.994,.995/,
5  X1(3,4),X1(3,5),X1(3,6)/.997,.998,.999/,
6  X1(4,1),X1(4,2),X1(4,3)/1.0,1.0,1.0/,
7  X1(4,4),X1(4,5),X1(4,6)/1.0,1.0,1.0/,
8  X1(5,1),X1(5,2),X1(5,3)/1.0,1.0,1.0/,
9  X1(5,4),X1(5,5),X1(5,6)/1.0,1.0,1.0/
  DATA X1(6,1),X1(6,2),X1(6,3)/1.0,1.0,1.0/,
1  X1(6,4),X1(6,5),X1(6,6)/1.0,1.0,1.0/,
2  X1(7,1),X1(7,2),X1(7,3)/1.0,1.0,1.0/,
3  X1(7,4),X1(7,5),X1(7,6)/1.0,1.0,1.0/,
4  X1(8,1),X1(8,2),X1(8,3)/1.0,1.0,1.0/,
5  X1(8,4),X1(8,5),X1(8,6)/1.0,1.0,1.0/,
6  X1(9,1),X1(9,2),X1(9,3)/1.0,1.0,1.0/,
7  X1(9,4),X1(9,5),X1(9,6)/1.0,1.0,1.0/
  DATA EF1(1,1),EF1(1,2),EF1(1,3),EF1(1,4)/1.121,1.154,1.173,1.211/,
1  EF1(1,5),EF1(1,6),EF1(2,1),EF1(2,2)/1.247,1.265,1.039,1.077/,
2  EF1(2,3),EF1(2,4),EF1(2,5),EF1(2,6)/1.114,1.117,1.149,1.173/,
3  EF1(3,1),EF1(3,2),EF1(3,3),EF1(3,4)/1.013,1.034,1.070,1.100/,
4  EF1(3,5),EF1(3,6),EF1(4,1),EF1(4,2)/1.129,1.168,1.020,1.058/,
5  EF1(4,3),EF1(4,4),EF1(4,5),EF1(4,6)/1.114,1.097,1.133,1.173/,
6  EF1(5,1),EF1(5,2),EF1(5,3),EF1(5,4)/1.021,1.076,1.158,1.224/,
7  EF1(5,5),EF1(5,6),EF1(6,1),EF1(6,2)/1.370,1.469,1.039,1.150/,
8  EF1(6,3),EF1(6,4),EF1(6,5),EF1(6,6)/1.212,1.312,1.441,1.572/,
9  EF1(7,1),EF1(7,2),EF1(7,3),EF1(7,4)/1.016,1.136,1.219,1.320/
  DATA EF1(7,5),EF1(7,6),EF1(8,1),EF1(8,2)/1.635,1.849,1.064,1.188/,
1  EF1(8,3),EF1(8,4),EF1(8,5),EF1(8,6)/1.309,1.462,1.548,2.050/,
2  EF1(9,1),EF1(9,2),EF1(9,3),EF1(9,4)/1.116,1.243,1.316,1.367/,
3  EF1(9,5),EF1(9,6)/1.564,1.533/

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READ THE TOTAL PRESSURE, MOLAR FRACTION OF ETHANE  
IN VAPOR PHASE AND LIQUID PHASE, EXPERIMENTAL  
ENHANCEMENT FACTOR

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  DATA P4(1,1),P4(1,2),P4(1,3)/34.01,47.62,61.22/,
1  P4(1,4),P4(1,5),P4(1,6)/68.03,102.44,136.05/,
2  P4(2,1),P4(2,2),P4(2,3)/15.22,34.01,47.62/,
3  P4(2,4),P4(2,5),P4(2,6)/61.22,102.44,136.05/,
4  P4(3,1),P4(3,2),P4(3,3)/24.9,40.9,60.1/,
5  P4(3,4),P4(3,5),P4(3,6)/90.7,120.2,143.5/,
7  P4(4,1),P4(4,2),P4(4,3)/17.01,34.01,47.62/,
8  P4(4,4),P4(4,5),P4(4,6)/61.22,102.44,136.05/
  DATA P4(5,1),P4(5,2),P4(5,3)/40.2,60.2,88.7/,
1  P4(5,4),P4(5,5),P4(5,6)/120.0,144.3,147.9/,
2  P4(6,1),P4(6,2),P4(6,3)/21.7,38.8,60.0/,
3  P4(6,4),P4(6,5),P4(6,6)/88.0,118.9,146.7/,
4  P4(7,1),P4(7,2),P4(7,3)/10.0,40.0,60.0/,
5  P4(7,4),P4(7,5),P4(7,6)/90.6,120.3,149.7/,
6  P4(8,1),P4(8,2),P4(8,3)/10.37,40.38,80.6/,
7  P4(8,4),P4(8,5),P4(8,6)/111.9,135.4,141.4/,
8  P4(9,1),P4(9,2),P4(9,3)/25.6,41.82,60.8/,

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9 P4(9,4),P4(9,5),P4(9,6)/83.6,110.0,144.2/  
 C DATA P4(10,1),P4(10,2),P4(10,3)/9.9,24.62,39.38/  
 C 1 P4(10,4),P4(10,5),P4(10,6)/69.4,108.2,148.0/  
 C 2 P4(11,1),P4(11,2),P4(11,3)/10.71,25.60,41.26/  
 C 3 P4(11,4),P4(11,5),P4(11,6)/70.6,106.5,149.1/  
 C 4 P4(12,1),P4(12,2),P4(12,3)/7.30,24.81,40.50/  
 C 5 P4(12,4),P4(12,5),P4(12,6)/71.0,109.6,149.1/  
 C  
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 C

DATA Y4(1,1),Y4(1,2)/524000.0,420000.0/  
 DATA Y4(1,3),Y4(1,4)/350000.0,320000.0/  
 1 Y4(1,5),Y4(1,6)/240000.0,220000.0/  
 2 Y4(2,1),Y4(2,2)/476000.0,240000.0/  
 3 Y4(2,3),Y4(2,4)/193000.0,170000.0/  
 4 Y4(2,5),Y4(2,6)/120000.0,104000.0/  
 5 Y4(3,1),Y4(3,2)/67300.0,46200.0/  
 6 Y4(3,3),Y4(3,4)/36000.0,29400.0/  
 7 Y4(3,5),Y4(3,6)/27000.0,26100.0/  
 8 Y4(4,1),Y4(4,2)/70000.0,43000.0/  
 9 Y4(4,3),Y4(4,4)/33000.0,25000.0/  
 DATA Y4(4,5),Y4(4,6)/20000.0,18000.0/  
 1 Y4(5,1),Y4(5,2)/15400.0,12400.0/  
 2 Y4(5,3),Y4(5,4)/11000.0,10500.0/  
 3 Y4(5,5),Y4(5,6)/10800.0,10600.0/  
 4 Y4(6,1),Y4(6,2)/5760.0,3890.0/  
 5 Y4(6,3),Y4(6,4)/3300.0,3100.0/  
 6 Y4(6,5),Y4(6,6)/3050.0,3310.0/  
 7 Y4(7,1),Y4(7,2)/1450.0,623.0/  
 8 Y4(7,3),Y4(7,4)/578.0,605.0/  
 9 Y4(7,5),Y4(7,6)/672.0,793.0/  
 DATA Y4(8,1),Y4(8,2)/554.0,269.0/  
 1 Y4(8,3),Y4(8,4)/276.0,325.0/  
 2 Y4(8,5),Y4(8,6)/381.0,395.0/  
 3 Y4(9,1),Y4(9,2),Y4(9,3)/65.1,39.2,42.6/  
 4 Y4(9,4),Y4(9,5),Y4(9,6)/53.3,70.0,101.0/  
 C 5 Y4(10,1),Y4(10,2),Y4(10,3)/5.7,4.13,4.36/  
 C 6 Y4(10,4),Y4(10,5),Y4(10,6)/6.94,13.7,24.0/  
 C 7 Y4(11,1),Y4(11,2),Y4(11,3)/.690,0.581,0.741/  
 C 8 Y4(11,4),Y4(11,5),Y4(11,6)/1.51,3.30,6.54/  
 C 9 Y4(12,1),Y4(12,2),Y4(12,3)/0.214,0.175,0.235/  
 C DATA Y4(12,4),Y4(12,5),Y4(12,6)/0.545,1.40,3.01/  
 C.....  
 C

DATA X4(1,1),X4(1,2),X4(1,3)/.98,.965,.95/  
 1 X4(1,4),X4(1,5),X4(1,6)/.94,.907,.873/  
 2 X4(2,1),X4(2,2),X4(2,3)/.99,.98,.968/  
 3 X4(2,4),X4(2,5),X4(2,6)/.958,.928,.90/  
 4 X4(3,1),X4(3,2),X4(3,3)/.98,.976,.9646/  
 5 X4(3,4),X4(3,5),X4(3,6)/.9484,.934,.9225/  
 6 X4(4,1),X4(4,2),X4(4,3)/.985,.98,.975/  
 7 X4(4,4),X4(4,5),X4(4,6)/.968,.95,.955/

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8   X4(5,1),X4(5,2),X4(5,3)/.9807,.9714,.9591/,
9   X4(5,4),X4(5,5),X4(5,6)/.9465,.938,.935/
  DATA X4(6,1),X4(6,2),X4(6,3)/.9915,.9851,.977/,
1   X4(6,4),X4(6,5),X4(6,6)/.967,.9586,.9493/,
2   X4(7,1),X4(7,2),X4(7,3)/.997,.9879,.9823/,
3   X4(7,4),X4(7,5),X4(7,6)/.9745,.9679,.96/,
4   X4(8,1),X4(8,2),X4(8,3)/.998,.9895,.981/,
5   X4(8,4),X4(8,5),X4(8,6)/.9745,.97,.9688/,
6   X4(9,1),X4(9,2),X4(9,3)/.995,.991,.988/,
7   X4(9,4),X4(9,5),X4(9,6)/.985,.9813,.976/
C   8   X4(10,1),X4(10,2),X4(10,3)/1.,1.,1./,
C   9   X4(10,4),X4(10,5),X4(10,6)/1.,1.,1./
C   DATA X4(11,1),X4(11,2),X4(11,3)/1.,1.,1./,
C   1   X4(11,4),X4(11,5),X4(11,6)/1.,1.,1./,
C   2   X4(12,1),X4(12,2),X4(12,3)/1.,1.,1./,
C   3   X4(12,4),X4(12,5),X4(12,6)/1.,1.,1./
  DATA EF4(1,1),EF4(1,2),EF4(1,3)/1.201,1.344,1.440/,
1   EF4(1,4),EF4(1,5),EF4(1,6)/1.500,1.791,2.10/,
2   EF4(2,1),EF4(2,2),EF4(2,3)/1.15,1.285,1.447/,
3   EF4(2,4),EF4(2,5),EF4(2,6)/1.6396,1.935,2.228/,
4   EF4(3,1),EF4(3,2),EF4(3,3)/1.29,1.45,1.66/,
5   EF4(3,4),EF4(3,5),EF4(3,6)/2.03,2.47,2.87/,
6   EF4(4,1),EF4(4,2),EF4(4,3)/1.104,1.356,1.457/,
7   EF4(4,4),EF4(4,5),EF4(4,6)/1.519,1.9,2.271/,
8   EF4(5,1),EF4(5,2),EF4(5,3)/1.53,1.84,2.4/,
9   EF4(5,4),EF4(5,5),EF4(5,6)/3.1,3.82,3.86/
  DATA EF4(6,1),EF4(6,2),EF4(6,3)/1.36,1.65,2.18/,
1   EF4(6,4),EF4(6,5),EF4(6,6)/2.96,3.99,5.23/,
2   EF4(7,1),EF4(7,2),EF4(7,3)/1.16,1.99,2.77/,
3   EF4(7,4),EF4(7,5),EF4(7,6)/4.37,6.45,9.47/,
4   EF4(8,1),EF4(8,2),EF4(8,3)/1.27,2.40,4.9/,
5   EF4(8,4),EF4(8,5),EF4(8,6)/8.03,11.4,12.3/,
6   EF4(9,1),EF4(9,2),EF4(9,3)/1.32,3.23,5.10/,
7   EF4(9,4),EF4(9,5),EF4(9,6)/8.78,15.2,28.5/
C   8   EF4(10,1),EF4(10,2),EF4(10,3)/1.62,2.92,4.92/,
C   9   EF4(10,4),EF4(10,5),EF4(10,6)/13.8,42.5,102.0/
C   DATA EF4(11,1),EF4(11,2)/1.93,3.88/,
C   1   EF4(11,3),EF4(11,4)/7.99,27.8/,
C   2   EF4(11,5),EF4(11,6)/91.7,255.0/,
C   3   EF4(12,1),EF4(12,2)/1.64,4.57/,
C   4   EF4(12,3),EF4(12,4)/10.0,40.7/,
C   5   EF4(12,5),EF4(12,6)/162.0,473.0/
C   READ THE THIRD VIRIAL COEFFICIENT OF KR
C   READ THE TOTAL PRESSURE, MOLAR FRACTION OF KR IN THE
C   VAPOR AND LIQUID PHASE, EXPERIMENTAL ENHANCEMENT FACTOR
  DATA P2(1,1),P2(1,2),P2(1,3)/10.17,20.18,40.29/,
1   P2(1,4),P2(1,5),P2(1,6)/90.9,100.0,120.8/,
2   P2(2,1),P2(2,2),P2(2,3)/9.89,10.22,20.2/,
3   P2(2,4),P2(2,5),P2(2,6)/39.92,79.4,117.7/,
4   P2(3,1),P2(3,2),P2(3,3)/4.73,10.07,20.1/,
5   P2(3,4),P2(3,5),P2(3,6)/41.60,79.0,119.0/

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6   P2(4,1),P2(4,2),P2(4,3)/9.8,20.0,39.89/,
7   P2(4,4),P2(4,5),P2(4,6)/79.5,81.2,120.0/,
8   P2(5,1),P2(5,2),P2(5,3)/2.62,20.0,39.85/,
9   P2(5,4),P2(5,5),P2(5,6)/79.4,80.6,115.5/
DATA P2(6,1),P2(6,2),P2(6,3)/4.2,20.2,40.28/,
1   P2(6,4),P2(6,5),P2(6,6)/64.6,80.4,106.6/,
2   P2(7,1),P2(7,2),P2(7,3)/4.02,10.09,20.04/,
3   P2(7,4),P2(7,5),P2(7,6)/39.9,80.0,105.0/,
4   P2(8,1),P2(8,2),P2(8,3)/4.1,10.0,19.82/,
5   P2(8,4),P2(8,5),P2(8,6)/39.3,59.8,90.0/,
6   P2(9,1),P2(9,2),P2(9,3)/10.0,19.6,37.6/,
7   P2(9,4),P2(9,5),P2(9,6)/59.9,79.3,80.7/
DATA Y2(1,1),Y2(1,2),Y2(1,3)/0.669,0.361,0.188/,
1   Y2(1,4),Y2(1,5),Y2(1,6)/.102,0.09,0.0715/,
2   Y2(2,1),Y2(2,2),Y2(2,3)/.416,0.395,0.213/,
3   Y2(2,4),Y2(2,5),Y2(2,6)/0.112,0.059,0.0437/,
4   Y2(3,1),Y2(3,2),Y2(3,3)/0.457,0.220,0.113/,
5   Y2(3,4),Y2(3,5),Y2(3,6)/0.0590,0.0339,0.025/,
6   Y2(4,1),Y2(4,2),Y2(4,3)/0.116,0.0595,0.032/,
7   Y2(4,4),Y2(4,5),Y2(4,6)/0.0182,0.0175,0.0133/,
8   Y2(5,1),Y2(5,2),Y2(5,3)/0.314,0.0451,0.0251/,
9   Y2(5,4),Y2(5,5),Y2(5,6)/0.0134,0.0132,0.00978/
DATA Y2(6,1),Y2(6,2),Y2(6,3)/0.164,0.0362,0.0193/,
1   Y2(6,4),Y2(6,5),Y2(6,6)/0.012,0.0106,0.00815/
DATA Y2(7,1),Y2(7,2),Y2(7,3)/.0997,0.042,0.0212/,
1   Y2(7,4),Y2(7,5),Y2(7,6)/.0114,.00653,.00535/,
2   Y2(8,1),Y2(8,2),Y2(8,3)/.0555,.0235,.012/,
3   Y2(8,4),Y2(8,5),Y2(8,6)/.0065,.00452,.00364/,
4   Y2(9,1),Y2(9,2),Y2(9,3)/.0121,.00363,.0025/,
5   Y2(9,4),Y2(9,5),Y2(9,6)/.0024,.0019,.00184/
DATA X2(1,1),X2(1,2),X2(1,3)/.9996,.998,.995/,
1   X2(1,4),X2(1,5),X2(1,6)/.9984,.986,.983/,
2   X2(2,1),X2(2,2),X2(2,3)/.9995,.9995,.9984/,
3   X2(2,4),X2(2,5),X2(2,6)/.9964,.9922,.9985/,
4   X2(3,1),X2(3,2),X2(3,3)/.9999,.9995,.999/,
5   X2(3,4),X2(3,5),X2(3,6)/.997,.995,.992/,
6   X2(4,1),X2(4,2),X2(4,3)/.9997,.9992,.9982/,
7   X2(4,4),X2(4,5),X2(4,6)/.9962,.99615,.994/,
8   X2(5,1),X2(5,2),X2(5,3)/.9999,.9992,.9985/,
9   X2(5,4),X2(5,5),X2(5,6)/.997,.997,.996/
DATA X2(6,1),X2(6,2),X2(6,3)/1.,1.,1./,
1   X2(6,4),X2(6,5),X2(6,6)/1.,1.,1./
DATA X2(7,1),X2(7,2),X2(7,3)/1.0,1.0,1.0/,
1   X2(7,4),X2(7,5),X2(7,6)/1.0,1.0,1.0/,
2   X2(8,1),X2(8,2),X2(8,3)/1.0,1.0,1.0/,
3   X2(8,4),X2(8,5),X2(8,6)/1.0,1.0,1.0/,
4   X2(9,1),X2(9,2),X2(9,3)/1.0,1.0,1.0/,
5   X2(9,4),X2(9,5),X2(9,6)/1.0,1.0,1.0/
DATA EF2(1,1),EF2(1,2),EF2(1,3)/1.05,1.12,1.17/,
1   EF2(1,4),EF2(1,5),EF2(1,6)/1.28,1.30,1.33/,
2   EF2(2,1),EF2(2,2),EF2(2,3)/1.07,1.08,1.15/,

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3  EF2(2,4),EF2(2,5),EF2(2,6)/1.19,1.25,1.37/,
4  EF2(3,1),EF2(3,2),EF2(3,3)/1.07,1.09,1.12/,
5  EF2(3,4),EF2(3,5),EF2(3,6)/1.21,1.32,1.46/,
6  EF2(4,1),EF2(4,2),EF2(4,3)/1.05,1.1,1.18/,
7  EF2(4,4),EF2(4,5),EF2(4,6)/1.34,1.31,1.47/,
8  EF2(5,1),EF2(5,2),EF2(5,3)/1.02,1.12,1.24/,
9  EF2(5,4),EF2(5,5),EF2(5,6)/1.32,1.32,1.4/,
DATA EF2(6,1),EF2(6,2),EF2(6,3)/1.03,1.09,1.16/,
1  EF2(6,4),EF2(6,5),EF2(6,6)/1.16,1.28,1.3/,
DATA EF2(7,1),EF2(7,2),EF2(7,3)/1.02,1.07,1.08/,
1  EF2(7,4),EF2(7,5),EF2(7,6)/1.15,1.32,1.42/,
2  EF2(8,1),EF2(8,2),EF2(8,3)/1.03,1.06,1.07/,
3  EF2(8,4),EF2(8,5),EF2(8,6)/1.15,1.22,1.31/,
4  EF2(9,1),EF2(9,2),EF2(9,3)/1.04,1.08,1.16/,
5  EF2(9,4),EF2(9,5),EF2(9,6)/1.23,1.30,1.26/

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C

C.....READ THE PRESS OF SYSTEM AND COMPOSITION

C

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DATA P3(1,1),P3(1,2),P3(1,3)/35.35,43.23,95.53/,
1  P3(1,4),P3(2,1),P3(2,2)/140.1,38.21,48.72/,
2  P3(2,4),P3(3,1),P3(3,2)/119.2,33.51,46.84/,
3  P3(3,4),P3(4,1),P3(4,2)/134.2,22.83,31.38/,
4  P3(2,3),P3(3,3),P3(4,4)/70.02,75.8,151.7/,
5  P3(4,3)/82.06/
DATA P3(5,1),P3(5,2),P3(5,3)/20.67,31.96,89.0/,
1  P3(6,1),P3(6,2),P3(6,3)/13.67,33.97,68.23/,
2  P3(7,1),P3(7,2),P3(7,3)/13.22,34.25,69.80/,
3  P3(5,4),P3(6,4),P3(7,4)/113.6,115.78,116.12/,
4  P3(8,1),P3(8,2),P3(8,3)/22.4,39.0,50.7/,
5  P3(8,4),P3(9,1),P3(9,2)/63.8,241.38,482.77/,
6  P3(9,3),P3(9,4)/965.55,965.55/
DATA Y3(1,1),Y3(1,2),Y3(1,3)/0.9002,.7973,.6079/,
1  Y3(2,1),Y3(2,2),Y3(2,3)/.6098,.5079,.3853/,
2  Y3(3,1),Y3(3,2),Y3(3,3)/.5079,.3853,.2624/,
3  Y3(4,1),Y3(4,2),Y3(4,3)/.5079,.3853,.1715/,
4  Y3(5,1),Y3(5,2),Y3(5,3)/.3853,.2624,.1103/,
5  Y3(6,1),Y3(6,2),Y3(6,3)/.247,.104,.0557/,
6  Y3(7,1),Y3(7,2),Y3(7,3)/.05,.0203,0.0111/,
7  Y3(1,4),Y3(2,4),Y3(3,4)/.385,.2624,.2624/,
8  Y3(4,4),Y3(5,4),Y3(6,4)/.110,.0919,.0379/,
9  Y3(7,4),Y3(8,1),Y3(8,2)/0.0085,0.0169,0.0105/
DATA Y3(8,3),Y3(8,4),Y3(9,1)/0.00862,0.00714,0.0016/,
1  Y3(9,2),Y3(9,3),Y3(9,4)/0.0018,0.0024,0.0024/

```

C

C

C

C

C

```

DATA X3(1,1),X3(1,2),X3(1,3)/.9926,.9827,.9316/,
1  X3(1,4),X3(2,1),X3(2,2)/.8683,.9817,.9717/,
2  X3(2,3),X3(2,4),X3(3,1)/.952,.908,.9817/,

```

```
3  X3(3,2),X3(3,3),X3(3,4)/.9728,.9496,.9052/,
4  X3(4,1),X3(4,2),X3(4,3)/.9906,.9728,.9496/,
5  X3(4,4),X3(5,1),X3(5,2)/.9026,.991,.9838/,
6  X3(5,3),X3(5,4),X3(6,1)/.9485,.934,.992/,
7  X3(6,2),X3(6,3),X3(6,4)/.9811,.944,.945/,
8  X3(7,1),X3(7,2),X3(7,3)/.996,.990,.97/,
9  X3(7,4),X3(8,1),X3(8,2)/.9615,.998,.991/
DATA X3(8,3),X3(8,4),X3(9,1)/.987,.987,1./,
1  X3(9,2),X3(9,3),X3(9,4)/1.,1.,1./
END
```

```

SUBROUTINE NAPO
C   SUBPROGRAM FOR CALCULATE THE SECOND VIRIAL COEFF.
C   USING THE KIHARA MODEL
C
DOUBLE PRECISION TET1,TET2,TET3,SET1,SET2,
1  SET3,PET1,PET2,PET3
DIMENSION ZUF(9),F3(9),F2(9),F1(9),R1(40),R2(40),R3(40)
COMMON /MAIN/ TEMPM(9),NT,NV,B(9),B11(9),B22(9),B12(9),
1  C111(9),C112(9),C122(9),C222(9),YVE(9,6),YV1(9,6),
2  YV2(9,6),TECE1,PRECTM,PEMTPM(9),UKV,
3  ANAV,DIS1,DIS2,PKM1,PKM2,SUR1,SUR2,VOLU1,VOLU2,
4  UNER1,UNER2,DIS,PKM,SUR,VOLU,UNER,TECE02,AMM1,
5  AMM2,XC1,XC2,VLC1,VLC2,EX,Y1(9,6),Y2(9,6),
6  Y3(9,6),Y4(9,6),X1(9,6),X2(9,6),X3(9,6),
7  X4(9,6),EF1(9,6),EF2(9,6),EF3(9,6),EF4(9,6),
8  NSYS,DEDO12
M=40
ANAV=.60238
PI=3.1416
C
C
REWIND 15
READ(15,7)(R1(J),R2(J),R3(J),J=1,M)
7  FORMAT(3E)
C
C   CALCULATE THE KIHARA PARAMETER
C
DO 80 I=1,NT
ZUF(I)=UNER1/TEMPM(I)
F1(I)=0.
F2(I)=0.
F3(I)=0.
C
DO 81 K=1,M
T=FLOAT(K)-1.
C   CALCULATE THE VALUE OF F1
TET1=(6.*T+1.)/12.0
TET2=ZUF(I)*TET1
TET3=R1(K)*TET2
F1(I)=F1(I)+TET3
C   CALCULATE THE VALUE OF F2
PET1=(6.*T+2.)/12.
PET2=ZUF(I)*PET1
PET3=R2(K)*PET2
F2(I)=F2(I)+PET3
C   CALCULATE THE VALUE OF F3
SET1=(6.*T+3.)/12.
SET2=ZUF(I)*SET1
SET3=R3(K)*SET2
F3(I)=F3(I)+SET3
81  CONTINUE
81

```

```
BE1=2.*PI*(DIS**3)*F3(I)/3.  
BE2=PKM*(DIS**2)*F2(I)  
BE3=(SUR+((PKM**2)/(4.*PI)))*DIS*F1(I)  
BE4=VOLU+((PKM*SUR)/(4.*PI))  
BE5=BE1+BE2+BE3+BE4  
B(I)=BE5*ANAV
```

```
80 CONTINUE  
RETURN  
END
```

```

SUBROUTINE PIPA
  DIMENSION ZUF(12),F3(12),F2(12),F1(12),R1(40),R2(40),R3(40)
C.....COMMON DATA
  COMMON /MAIN/ TEMPM(9),NT,NV,B(9),B11(9),B22(9),B12(9),
1  C111(9),C112(9),C122(9),C222(9),YVE(9,6),YV1(9,6),
2  YV2(9,6),TECE1,PRECTM,PEMTPM(9),UKV,
3  ANAV,DIS1,DIS2,PKM1,PKM2,SUR1,SUR2,VOLU1,VOLU2,
4  UNER1,UNER2,DIS,PKM,SUR,VOLU,UNER,TECE02,AMM1,
5  AMM2,XC1,XC2,VLC1,VLC2,EX,Y1(9,6),Y2(9,6),
6  Y3(9,6),Y4(9,6),X1(9,6),X2(9,6),X3(9,6),
7  X4(9,6),EF1(9,6),EF2(9,6),EF3(9,6),EF4(9,6),
8  NSYS,DEDO12
  M=40
  PI=3.1416
  REWIND 15
  READ(15,7)(R1(J),R2(J),R3(J),J=1,M)
7  FORMAT(3E)
  DO 90 I=1,NT
    DIS12=(DIS1+DIS2)*0.5
    UNER12=(UNER1*UNER2)**0.5*(1.- UKV)
    ZUF(I)=UNER12/TEMPM(I)
C.....CALCULATE THE VALUE OF KIHARA PARAMETER
    F1(I)=0.
    F2(I)=0.
    F3(I)=0.
    EXI=1.00E-10
    DO 91 K=1,M
      P=FLOAT(K)-1.
C.....CALCULATE THE VALUE OF F1
      TET1=(6.*P+1.)/12.0
      TET2=ZUF(I)**TET1
      TET3=R1(K)*TET2
      IF(TET2.LE.EXI) GO TO 201
      F1(I)=F1(I)+TET3
C.....CALCULATE THE VALUE OF F2
201    PET1=(6.*P+2.)/12.0
      PET2=ZUF(I)**PET1
      PET3=R2(K)*PET2
      IF(PET2.LE.EXI) GO TO 202
      F2(I)=F2(I)+PET3
C.....CALCULATE THE VALUE OF F3
202    SET1=(6.*P+3.)/12.0
      SET2=ZUF(I)**SET1
      SET3=R3(K)*SET2
      IF(SET2.LE.EXI) GO TO 91
      F3(I)=F3(I)+SET3
91  CONTINUE
    BE1=2.*PI*DIS12**3*F3(I)/3.
    BE2=(PKM1+PKM2)/(2.)*DIS12**2*F2(I)
    BE3=((SUR1+SUR2)/(2.)+(PKM1*PKM2)/(4.*PI))*DIS12*F1(I)
    BE4=(VOLU1+VOLU2)/(2.)+(PKM1*SUR2+PKM2*SUR1)/(8.*PI)

```

```
      BE5=BE1+BE2+BE3+BE4  
      B12(I)=BE5*ANAV  
90    CONTINUE  
      RETURN  
      END
```

## SUBROUTINE LIRA

```

DIMENSION TECE12(12),TRR(12),C4(9,6),C12(9)
COMMON /MAIN/ TEMPM(9),NT,NV,B(9),B11(9),B22(9),B12(9),
1  C111(9),C112(9),C122(9),C222(9),YVE(9,6),YV1(9,6),
2  YV2(9,6),TECE1,PRECTM,PEMTPM(9),UKV,
3  ANAV,DIS1,DIS2,PKM1,PKM2,SUR1,SUR2,VOLU1,VOLU2,
4  UNER1,UNER2,DIS,PKM,SUR,VOLU,UNER,TECE02,AMM1,
5  AMM2,XC1,XC2,VLC1,VLC2,EX,Y1(9,6),Y2(9,6),
6  Y3(9,6),Y4(9,6),X1(9,6),X2(9,6),X3(9,6),
7  X4(9,6),EF1(9,6),EF2(9,6),EF3(9,6),EF4(9,6),
8  NSYS,DEDO12

```

```
XC1=21.8
```

```
XC2=-9.91
```

```
DO 500 J=1,NT
```

```
TEC2=TECE02/(1. + XC1/(AMM2*TEMPM(J)))
```

```
VC2=VLC2/(1. + XC2/(AMM2*TEMPM(J)))
```

```
TECE12(J)=((TEC2*TECE1)**0.5)*(1. - UKV)
```

```
TRR(J)=TEMPM(J)/TECE12(J)
```

```
IF(TRR(J).GT.1.75)DEDO12=0.0
```

```
VLC12=((VLC1**0.333 + VC2**0.333)*0.5)**3
```

```
AK5=0.232/(TRR(J)**0.25)
```

```
AK6=0.468/(TRR(J)**5)
```

```
AK7=1.-1.89*TRR(J)**2
```

```
IF(AK7.LT.1.E-16)AK7=1.E-15
```

```
AK8=2.49-2.30*TRR(J)+2.7*TRR(J)**2
```

```
IF(AK8.GT.16)AK8=15.
```

```
AK9=((AK5+AK6)*(1.-EXP(AK7)))+DEDO12*EXP(-AK8)
```

```
C12(J)=AK9*VLC12**2
```

```
C112(J)=(C111(J)*C12(J)**2)**0.333
```

```
C122(J)=(C222(J)*C12(J)**2)**0.333
```

```
IF(NSYS.EQ.3)NV=4
```

```
DO 510 L=1,NV
```

```
IF(NSYS.EQ.1)YVE(J,L)=Y1(J,L)
```

```
IF(NSYS.EQ.2)YVE(J,L)=Y2(J,L)
```

```
IF(NSYS.EQ.3)YVE(J,L)=Y3(J,L)
```

```
IF(NSYS.EQ.4)YVE(J,L)=Y4(J,L)
```

```
YV1(J,L)=YVE(J,L)/EX
```

```
YV2(J,L)=(EX-YVE(J,L))/EX
```

```
BK1=YV1(J,L)**3*C111(J)
```

```
BK2=3.*YV1(J,L)**2*YV2(J,L)*C112(J)
```

```
BK3=3.*YV1(J,L)*YV2(J,L)**2*C122(J)
```

```
BK4=YV2(J,L)**3.*C222(J)
```

```
C4(J,L)=BK1+BK2+BK3+BK4
```

```
510 CONTINUE
```

```
500 CONTINUE
```

```
RETURN
```

```
END
```

A P P E N D I X   B

TABLE B1 KIHARA POTENTIAL PARAMETERS

Substance	$\rho_0 \text{ \AA}$	$M_0 \text{ \AA}$	$S_0 \text{ \AA}^2$	$V_0 \text{ \AA}^3$	$U_0/k \text{ } ^\circ\text{K}$	Ref
Helium	2.921	0.0	0.0	0.0	9.9	[6]
Kr	3.483	2.639	0.554	0.038	212.38	[6]
H <sub>2</sub>	2.808	2.32	0.0	0.0	46.0	[6]
C <sub>6</sub> H <sub>6</sub>	3.4	13.1	10.04	6.256	832.0	[14]
C <sub>2</sub> H <sub>6</sub>	2.840	10.17	5.77	.653	444.0	[6]

TABLE B2. KIHARA COEFFICIENTS

+1.055546E+00,	+1.123737E+00,	+1.225415E+00
-3.545929E-01,	-3.929795E-01,	-1.312905E-00
-1.759244E-01,	-3.762623E-01,	-6.127093E-01
-9.949800E-02,	-1.924399E-01,	-3.021341E-01
-5.375469E-02,	-1.045173E-01,	-2.531771E-01
-2.790777E-02,	-5.291730E-02,	-7.553353E-02
-1.373731E-02,	-2.554267E-02,	-1.574132E-02
-6.423216E-03,	-1.175940E-02,	-1.413576E-02
-2.861939E-03,	-5.170565E-03,	-7.020616E-03
-1.219221E-03,	-2.177657E-03,	-2.922629E-03
-4.901893E-04,	-3.309110E-04,	-1.170103E-03
-1.956144E-04,	-3.431474E-04,	-4.516430E-04
-7.422517E-05,	-1.231223E-04,	-1.624233E-04
-2.719644E-05,	-4.692614E-05,	-6.079876E-05
-9.651992E-06,	-1.654132E-05,	-2.173434E-05
-3.324000E-06,	-5.560332E-06,	-7.237249E-06
-1.112660E-06,	-1.583373E-06,	-2.394489E-06
-3.625451E-07,	-6.104927E-07,	-7.716931E-07
-1.151446E-07,	-1.929220E-07,	-2.455739E-07
-3.563914E-08,	-5.950222E-08,	-7.446152E-08
-1.090743E-08,	-1.793650E-08,	-2.234279E-08
-3.201698E-09,	-3.299322E-09,	-6.559716E-09
-9.279094E-10,	-1.527061E-09,	-1.896080E-09
-2.635613E-10,	-4.320463E-10,	-5.315194E-10
-7.340346E-11,	-1.193730E-10,	-1.463223E-10
-2.005994E-11,	-3.264349E-11,	-3.936333E-11
-5.382919E-12,	-3.729574E-12,	-1.042365E-11
-1.413245E-12,	-2.294034E-12,	-2.722521E-12
-3.678303E-13,	-5.927468E-13,	-7.166750E-13
-9.330073E-14,	-1.505755E-13,	-1.916173E-13
-2.353870E-14,	-3.763373E-14,	-4.530704E-14
-5.616316E-15,	-9.233355E-15,	-1.113141E-14
-1.415302E-15,	-2.254390E-15,	-2.694673E-15
-3.386523E-16,	-5.395100E-16,	-6.431077E-16
-8.033915E-17,	-1.272814E-16,	-1.513052E-16
-1.874272E-17,	-2.952016E-17,	-3.512227E-17
-4.314456E-18,	-6.821308E-18,	-8.045593E-18
-9.802870E-19,	-1.541790E-18,	-1.819397E-18
-2.199165E-19,	-3.450393E-19,	-4.062952E-19
-4.872771E-20,	-7.629130E-20,	-8.961341E-20

A P P E N D I X C

TABLE C1. VIRIAL COEFFICIENTS FOR He-C<sub>2</sub>H<sub>6</sub> SYSTEM

TEMP(K)	B11 (*)	B22 (*)	B12 (*)	C111 (**)	C222 (**)	C122 (**)	C112 (**)
230.00	-0.31E+03	0.12E+02	0.24E+02	0.35E+02	0.19E+03	0.54E+03	0.31E+03
200.00	-0.42E+03	0.12E+02	0.22E+02	-0.10E+03	0.19E+03	0.56E+03	-0.45E+03
170.00	-0.58E+03	0.12E+02	0.19E+02	-0.64E+03	0.19E+03	0.57E+03	-0.86E+03
150.00	-0.77E+03	0.12E+02	0.16E+02	-0.18E+04	0.19E+03	0.59E+03	-0.12E+04
130.00	-0.11E+04	0.12E+02	0.13E+02	-0.50E+04	0.20E+03	0.61E+03	-0.18E+04
122.00	-0.13E+04	0.11E+02	0.11E+02	-0.77E+04	0.20E+03	0.62E+03	-0.21E+04
112.00	-0.16E+04	0.11E+02	0.80E+01	-0.14E+05	0.20E+03	0.63E+03	-0.26E+04
102.00	-0.21E+04	0.11E+02	0.45E+01	-0.26E+05	0.20E+03	0.64E+03	-0.32E+04
95.00	-0.25E+04	0.11E+02	0.16E+01	-0.41E+05	0.20E+03	0.65E+03	-0.38E+04

(\*) (cm<sup>3</sup>/g mole)      (\*\*) (cm<sup>3</sup>/g mole)<sup>2</sup>

TABLE C2. VIRIAL COEFFICIENTS FOR He-Kr SYSTEM

TEMP(K)	B11 (*)	B22 (*)	B12 (*)	C111 (**)	C222 (**)	C122 (**)	C112 (**)
150.00	-0.20E+03	0.12E+02	0.11E+02	0.35E+02	0.19E+03	0.40E+03	0.23E+03
140.00	-0.23E+03	0.12E+02	0.97E+01	0.45E+02	0.20E+03	0.41E+03	0.25E+03
130.00	-0.26E+03	0.12E+02	0.82E+01	0.59E+02	0.20E+03	0.41E+03	0.28E+03
120.85	-0.30E+03	0.11E+02	0.66E+01	0.76E+02	0.20E+03	0.42E+03	0.30E+03
117.09	-0.32E+03	0.11E+02	0.58E+01	0.87E+02	0.20E+03	0.42E+03	0.32E+03
115.00	-0.33E+03	0.11E+02	0.54E+01	0.92E+02	0.20E+03	0.42E+03	0.33E+03
110.00	-0.36E+03	0.11E+02	0.47E+01	0.12E+03	0.20E+03	0.43E+03	0.36E+03
105.00	-0.40E+03	0.11E+02	-0.66E+02	0.14E+03	0.20E+03	0.43E+03	0.39E+03
100.00	-0.44E+03	0.11E+02	0.40E+00	0.16E+03	0.20E+03	0.43E+03	0.41E+03
(*)	(cm <sup>3</sup> /gmole)	(**)	(cm <sup>3</sup> /gmole) <sup>2</sup>				

TABLE C3. VIRIAL COEFFICIENTS FOR H<sub>2</sub>-C<sub>6</sub>H<sub>6</sub> SYSTEM

TEMP(K)	B11 (*)	B22 (*)	B12 (*)	C111 (**)	C222 (**)	C122 (**)	C112 (**)
523.16	-0.39E+03	0.17E+02	0.38E+02	0.23E+02	0.27E+03	0.12E+04	0.52E+03
493.16	-0.44E+03	0.16E+02	0.37E+02	0.29E+02	0.27E+03	0.12E+04	0.56E+03
473.16	-0.48E+03	0.16E+02	0.36E+02	0.34E+02	0.27E+03	0.12E+04	0.60E+03
453.16	-0.53E+03	0.16E+02	0.34E+02	0.41E+02	0.27E+03	0.12E+04	0.64E+03
433.16	-0.59E+03	0.16E+02	0.33E+02	0.50E+02	0.28E+03	0.12E+04	0.69E+03
394.27	-0.73E+03	0.16E+02	0.30E+02	0.88E+02	0.28E+03	0.12E+04	0.85E+03
338.72	-0.10E+04	0.15E+02	0.24E+02	0.12E+03	0.20E+03	0.13E+04	0.96E+03
323.16	-0.12E+04	0.15E+02	0.21E+02	0.13E+03	0.29E+03	0.13E+04	0.97E+03
298.16	-0.14E+04	0.14E+02	0.17E+02	0.15E+03	0.29E+03	0.13E+04	0.11E+04

(\*) (cm<sup>3</sup>/g mole)      (\*\*) (cm<sup>3</sup>/g mole)<sup>2</sup>

TABLE C4. VIRIAL COEFFICIENTS FOR H<sub>2</sub>-C<sub>2</sub>H<sub>6</sub> SYSTEM

TEMP(K)	B11 (*)	B22 (*)	B12 (*)	C111 (**)	C222 (**)	C122 (**)	C112 (**)
255.30	-0.25E+03	0.13E+02	-0.48E+01	0.66E+02	0.30E+03	0.92E+03	0.55E+03
227.60	-0.32E+03	0.12E+02	-0.12E+02	0.30E+02	0.31E+03	0.95E+03	0.44E+03
189.47	-0.46E+03	0.10E+02	-0.26E+02	-0.27E+03	0.31E+03	0.10E+04	-0.91E+03
186.00	-0.48E+03	0.10E+02	-0.27E+02	-0.27E+03	0.31E+03	0.10E+04	-0.99E+03
169.40	-0.59E+03	0.87E+01	-0.36E+02	-0.66E+03	0.32E+03	0.11E+04	-0.14E+04
149.62	-0.77E+03	0.68E+01	-0.50E+02	-0.18E+04	0.33E+03	0.12E+04	-0.21E+04
130.00	-0.11E+04	0.42E+01	-0.70E+02	-0.50E+04	0.34E+03	0.14E+04	-0.33E+04
122.00	-0.13E+04	0.29E+01	-0.80E+02	-0.77E+04	0.34E+03	0.14E+04	-0.41E+04
108.00	-0.18E+04	0.25E-01	-0.10E+03	-0.18E+05	0.36E+03	0.16E+04	-0.59E+04
95.00	-0.25E+04	-0.36E+01	-0.14E+03	-0.41E+05	0.38E+03	0.17E+04	-0.82E+04
87.00	-0.34E+04	-0.64E+01	-0.16E+03	-0.72E+05	0.40E+03	0.17E+04	-0.94E+04
83.00	-0.39E+04	-0.80E+01	-0.18E+03	-0.97E+05	0.41E+03	0.15E+04	-0.94E+04

(\*) (cm<sup>3</sup>/g mole)      (\*\*) (cm<sup>3</sup>/g mole)<sup>2</sup>