Int. J. Heat Mass Transfer. Vol. 11, pp. 1771–1778. Pergamon Press 1968. Printed in Great Britain

UNLIKE INTERACTIONS AND BINARY DIFFUSION IN POLAR–NONPOLAR MIXTURES; KRYPTON–METHYLENE CHLORIDE AND KRYPTON–ETHYLCHLORIDE

YASHWANT SINGH and B. N. SRIVASTAVA
Indian Association for the Cultivation of Science, Calcutta-32, India

(*Received* 7 *October* 1967)

Abstract—Binary diffusion coefficients of gases having one polar constituent have been measured in the temperature range 275 to 318°K using the two-bulb technique of Ney and Armistead. The systems investigated were Kr–CH_2Cl_2 and Kr–C_2H_5Cl. Radioactive ^{85}Kr was used as a tracer and a scintillation counter was employed to determine its concentration at different times. The mass correction was applied to get the normal diffusion coefficients for both the systems.

The experimental D_{12} values have been employed to get the unlike interaction parameters on the Lennard–Jones (12:6) potential and compared with those obtained by using the combination rules for a polar–nonpolar system and the force constants of the polar gas from viscosity as well as from second virial data. The off-centre model of Blanks and Prausnitz is discussed in detail.

NOMENCLATURE

A,	cross section area [cm^2];
$B(T)$,	second virial coefficient [$cm^3 mol^{-1}$];
C_1,	concentration of reference gas;
D,	diffusion coefficient [$cm^2 s^{-1}$];
I,	ionization potential [eV];
k,	Boltzmann constant [erg °C^{-1}];
K_j,	correction term in equation (9) due the off-centre nature of dipole;
l,	effective diffusion path [cm];
N_1,	number of counts;
p,	pressure [cmHg];
r,	intermolecular distance;
t,	time [s];
T,	temperature [°K];
V,	volume [cm^3];
V_{cj},	critical volume of polar molecule [$cm^3 mol^{-1}$].

Greek symbols

α,	polarizability [cm^3];
ϵ, σ,	molecular force parameters;
η,	viscosity coefficient [$g . cm^{-1} . s^{-1}$];
λ,	thermal conductivity coefficient [$cal . cm^{-1} . s^{-1} . degC^{-1}$];
μ_j,	dipole moment [D];
μ_{12},	reduced mass;
ξ,	correction term in equations (3) and (4) given by equation (5);
τ,	relaxation time [s];
$\varphi(r)$,	intermolecular potential energy [erg].

Subscripts

1, 2,	species of molecules;
i,	nonpolar molecule;
ii,	nonpolar–nonpolar interaction;
ij,	nonpolar–polar interaction;
j,	polar molecule;
jj,	polar–polar interaction;
$jj(np)$,	nonpolar interaction of polar molecule.

Superscripts

*,	quantity reduced by means of simplest

combination of molecular parameters σ and ϵ;

$\dagger$, quantity reduced by means of combination of σ and ϵ which utilize rigid sphere value.

INTRODUCTION

THE POTENTIAL function which describes the intermolecular forces between a polar and a nonpolar but polarizable molecule is commonly written as the sum of three parts; the first consider the forces of repulsion which vary as the inverse twelfth power of the distance between molecular centres, the second considers dispersion forces due to the polarizability of both molecules and the third considers the forces of induction which result from the dipole induced in the nonpolar molecule by the polar molecule. The last two parts of the potential function vary as inverse sixth power of the intermolecular distance. It is thus possible to write the potential between a nonpolar molecule i and a polar molecule j on Lennard–Jones (12:6) form

$$\varphi(r) = 4\epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r}\right)^{12} - \left(\frac{\sigma_{ij}}{r}\right)^{6}\right] \tag{1}$$

where ϵ_{ij} is the depth of the potential and σ_{ij} is the value of r for which $\varphi(r) = 0$. These force parameters can be derived from a knowledge of the binary diffusion coefficients or vice versa.

According to Chapman–Enskog theory [1] the general expression for the diffusion coefficient D_{12} of a binary gas mixture in the first approximation is given by

$$[D_{12}]_1 = \frac{3}{8\sqrt{\pi}} \cdot \frac{\sqrt{(k^3T^3/2\mu_{12})}}{\sigma_{12}^2\Omega_{12}^{(11)\dagger}(T_{12}^*)} \cdot \frac{1}{p}. \tag{2}$$

In this expression p, T and μ denote pressure, temperature and reduced mass respectively; k is the Boltzmann constant, the subscripts 1 and 2 refer to molecules of species 1 and 2. The intermolecular potential model enters equation (2) through σ_{12} and $\Omega^{(11)\dagger}$ with $T_{12}^* = kT/\epsilon_{12}$. $\Omega^{(11)\dagger}$ is the diffusion collision integral reduced in the usual way [1]. As the right-hand side of equation (2) depends only on the properties of unlike interactions, the first Chapman–Enskog approximation of D_{12} is very suitable for getting information on σ_{12} and ϵ_{12}.

The forces between a pair of unlike molecules could also be estimated from those between the corresponding pair of like molecules by using the proper combination rules. The most commonly used semiemperical combining rules for a pair of unlike molecules are due to Blanks and Prausnitz [2].

$$\sigma_{ij} = \frac{\sigma_{ii} + \sigma_{jj}}{2}[1 + \xi_{ij}]^{-\frac{1}{6}} \tag{3}$$

$$\epsilon_{ij} = (\epsilon_{ii}\epsilon_{jj})^{\frac{1}{2}}[1 + \xi_{ij}]^2 \tag{4}$$

in which

$$\xi_{ij} = \frac{\alpha_i\mu_j^2}{4\left[\dfrac{\sigma_{ii} + \sigma_{jj}}{2}\right]^6 (\epsilon_{ii}\epsilon_{jj})^{\frac{1}{2}}} \tag{5}$$

where σ_{ii}, ϵ_{ii} are the Lennard–Jones potential parameters for nonpolar molecules, σ_{jj}, ϵ_{jj} the Stockmayer potential parameters for polar molecules, α_i, the polarizability of the nonpolar molecule and μ_j, the dipole moment of the polar molecule.

The present paper reports a continuation of attempts to obtain information on the forces between unlike molecules (in polar–nonpolar mixtures) by studying diffusion in binary gas mixtures. While viscosity η and thermal conductivity λ depend on both like and unlike interactions, the diffusion coefficient D, in the first approximation, depends directly and sensitively on the forces between unlike molecules and thus are of particular interest for this purpose. Accordingly, the experimental measurements of binary diffusion in polar–nonpolar mixture have been of particular interest in recent years [3–6].

Recently Srivastava and Saran [6, 7] have studied the mutual diffusion coefficient in the mixture of Kr and a few polar gases by using radioactive ^{85}Kr as tracer. They have observed that the force parameters for the polar gases as obtained from viscosity by Monchick and Mason [8] and used in conjunction with above combining laws represent the observed D_{12} values fairly well. But when the force parameters are taken from $B(T)$ data [9] and used in conjunction with the combining laws, the calculated values are much higher. However, by considering the off-centre dipole model of Blanks and Prausnitz [2] they found that the second virial data also yield reasonable unlike force parameters. In the present investigation we have chosen the strongly polar gases methylene chloride and ethyl chloride to examine their behaviour in polar–nonpolar gas mixture. The behaviour of ethyl chloride is interesting in the sense that the value of σ obtained from $B(T)$ data is larger than that obtained from viscosity data in contradiction to other polar gases [2].

PRINCIPLES AND THEORY

The detailed theory of diffusion in the two bulb apparatus has been worked out by Ney and Armistead [10] and it has been shown that for the geometry of the apparatus employed in present investigation, the relaxation time α of the system as defined by the relation

$$(C_1^t - C_1^\infty)/(C_1^0 - C_1^\infty) = \exp(-\alpha t) \tag{6}$$

is given by

$$\tau = \frac{1}{\alpha} = \left(\frac{l}{D_p \times A}\right)\left(\frac{V_1 V_2}{V_0}\right) \tag{7}$$

where C_1^0, C_1^t and C_1^∞ respectively denote the concentration of the reference gas in the analysing chamber initially, after t s, and after complete mixing. The value of C_1^∞ is found from the geometry of the apparatus and the initial concentration and also checked experimentally; V_1 and V_2 are the volume of the analysing and other chamber in cm^3, V_0 being $V_1 + V_2$. D_p is the binary diffusion coefficient in cm^2/s at a pressure of p cmHg. A and l are the cross-sectional area and effective diffusion path respectively. Since the concentration C_1 in equation (6) occurs both in numerator and denominator, it is possible to determine the relaxation time of the system by knowing only the relative concentrations rather than their absolute values. The number of counts N_1 recorded at the window of the analysing chamber is proportional to the concentration of the radioactive component in the chamber. The relaxation time τ corresponding to $\log_{10}[(N_1^0 - N_1^\infty)/e]$ is read directly from the plot of $\log_{10}[N_1^t - N_1^\infty]$ vs. time t, which gives a straight line. N_1^0, N_1^t and N_1^∞ respectively denote the count initially, at t s and after complete mixing. The diffusion coefficient D_{atm} at atmospheric pressure is related to D_p through the relation

$$D_{\text{atm}} = D_p(p/1\ \text{atm}). \tag{8}$$

A mass correction is then applied to obtain the binary diffusion coefficient.

EXPERIMENTAL

Apparatus and procedure

The detail of the apparatus and the experimental procedure have already been discussed by Srivastava and Paul [11] and Srivastava and Saran [6]. The experiment was begun by equalizing the gas pressure in both chamber and opening the capillary valve connecting the bulbs. The whole assembly was immersed in a water bath in which the temperature was controlled to better than 0·05 degC by Sunvic electronic relay. For each run at any temperature, diffusion proceeded for about 2 h. The counts were taken for 1 min at intervals of 5 min. All the readings were corrected for background constant and counting loss in the scintillation counter.

The constants of the apparatus are as follows:

volume of the analysing chamber = 197·3 cm^3
volume of the other chamber = 184·3 cm^3
length of the capillary = 8·058 cm
diameter of the capillary = 0·306 cm
C_1^∞ = 0·517.

The experiments were carried out in the temperature range 273–318°K and the pressure in the range 15–24 mm of mercury. The higher temperature limit was set by the limitation of the scintillation crystal and the lower limit by the liquefaction of the gas.

Preparation of gases

Pure and dry methylene chloride vapour was prepared by the method already described by Srivastava and Srivastava [12], with a tower filled with fused calcium chloride. Pure liquid methylene chloride supplied by E. Merck, Germany was used and the vapour was collected in a gas cylinder having a metal stopcock at a pressure of about 30 cm of mercury. A similar apparatus was utilized for collecting the ethyl chloride vapour with a cooling arrangement attached to the funnel. The vapours were further purified by fractionation at liquid nitrogen temperature. The liquid ethyl chloride was supplied by Gebr. Eichhorn, Germany in lever locked tube.

Experimental results

The determination of relaxation time τ as defined by equation (6) is displayed in Figs. 1 and 2 where $\log_{10}(N_1^t - N_1^\infty)$ is plotted against t for the two mixtures at two temperatures. The relaxation time τ for the system at the experimental pressure p is obtained directly from the plot. The value of τ is used to calculate D_p from equation (7). Experimental values of p, D_p and D_{atm} are recorded in Table 1. No other experimental data for these systems are available for comparison. We believe our data to be accurate within ±1 per cent.

Determination of potential parameters

The intersection method of Buckingham [12] has been employed to get the unlike interaction parameters for the systems considered here on Lennard–Jones (12:1) model. It has been shown that the effective energy of interaction between a polar and a nonpolar molecule has the same form as that between two nonpolar molecules. The diffusion collision integrals $\Omega^{(11)\dagger}$ on 12:6 model are tabulated as a function of T^* by Hirschfelder *et al.* [1]. The force constants determined by fitting the observed D_{12} values are given in Table 2.

The unlike interaction parameters obtained

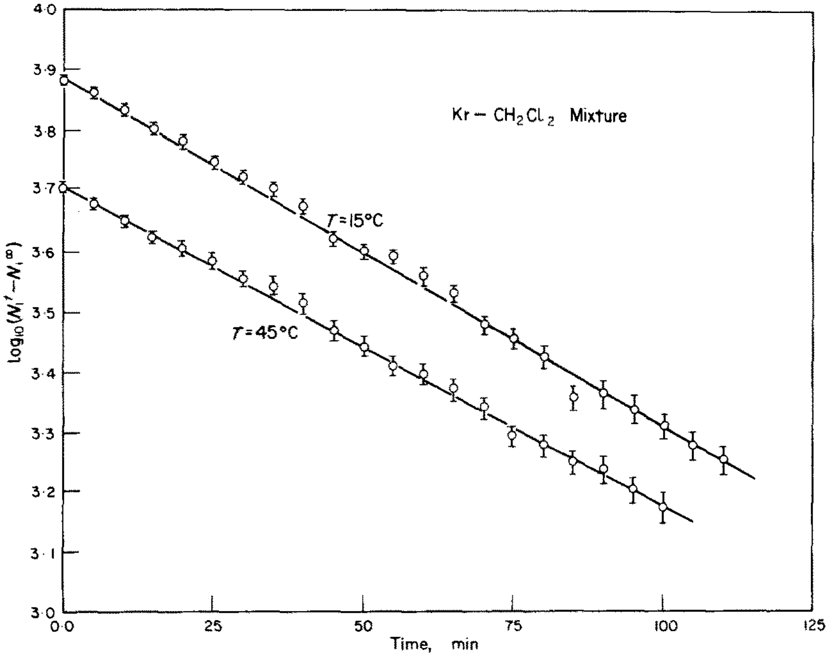

FIG. 1. The plot of $\log_{10}(N_1^t - N_1^\infty)$ vs. time for the Kr–CH$_2$Cl$_2$ mixture.

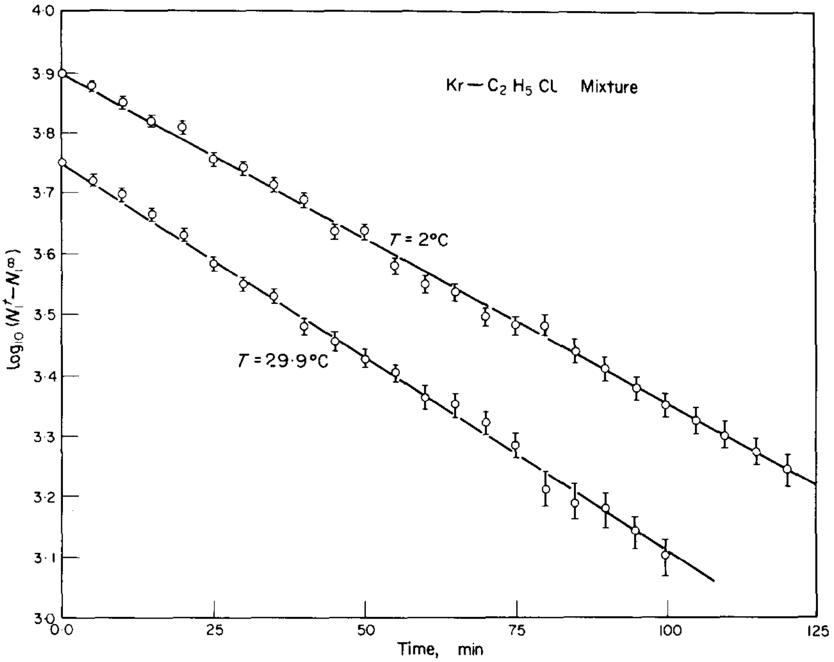

FIG. 2. The plot of $\log_{10}(N'_1 - N_1^{\infty})$ vs. time for the Kr–C_2H_5Cl mixture.

Table 1. Mutual diffusion coefficient in cm^2/s

Gas mixture	T °K	Pressure (mm Hg)	D_p	D_{atm}				
				Experimental	(a)	(b)	(c)	(d)
Kr–CH_2Cl_2	278·4	15·78	2·485	0·0518	0·0517	0·0537	0·0671	
	288·2	18·46	2·274	0·0554	0·0555	0·0575	0·0720	
	303·2	20·84	2·244	0·0613	0·0614	0·0636	0·0797	
	318·2	23·82	2·147	0·0675	0·0675	0·0699	0·0878	
Kr–C_2H_5Cl	275·2	20·85	2·161	0·0595	0·0597	0·0592	0·0508	0·0663
	288·2	27·62	1·988	0·0653	0·0654	0·0648	0·0556	0·0723
	303·2	21·11	2·577	0·0720	0·0722	0·0717	0·0614	0·0795
	318·2	23·69	2·539	0·0794	0·0793	0·0788	0·0674	0·0869

(a) Calculated from the force constants fitted to D_{12} data.

(b) Calculated from the combination rules and the force constants of the polar gas from the viscosity.

(c) Calculated from the combination rules and the force constants of the polar gas from $B(T)$ data.

(d) Calculated from the force constants for the polar gas obtained by the method of Blanks and Prausnitz and utilizing their empirical combination rules for interaction between a noncentral dipole and a nonpolar molecule.

by using the combination rules (equations (3–5)) and the force constants for the polar gases taken from the viscosity [8] data for the system investigated here are recorded in column four of Table 2. The force parameters for Kr are those determined by Clifton [13] from his recent viscosity measurements and are in reasonable agreement with the values derived from recent virial coefficient measurements [14]. The unlike interaction parameters have also been obtained by taking the force constants of polar gases from $B(T)$ data and these are recorded in column 5

Table 2. Potential parameters for the Lennard–Jones (12:6) model

Gas mixture	Force parameters	Present work (from D_{12} values)	Combining laws		
			(a)	(b)	(c)
Kr–CH_2Cl_2	$\epsilon_{12/k}$ °K	302	284·3	342·5	
	σ_{12} Å	4·139	4·126	3·518	
Kr–C_2H_5Cl	$\epsilon_{12/k}$ °K	250	269·7	231·7	163·0
	σ_{12} Å	4·138	4·082	4·565	4·306

(a) Using the force constants for the polar gas from viscosity.
(b) Using the force constants for the polar gas from $B(T)$ data.
(c) Using the force constants for the polar gas obtained by the method of Blanks and Prausnitz and utilizing their combination rules for interaction between a non-central dipole and nonpolar molecule.

of Table 2. We have determined the force constants for CH_2Cl_2(ϵ/k = 700°K, σ = 3·322 Å) from the $B(T)$ data of Perez Masiá and Diaz Peña [15] and those for C_2H_5Cl (ϵ/k = 320 and σ = 5·41 Å) are those given by Rowlinson [9].

DISCUSSION

The calculated values of D_{12} from the three sets of force constants (recorded in Table 2) are compared with the experimental D_{12} values in Table 1. Agreement between the experimental values for D_{12} and the values calculated from the (experimentally determined) unlike force constants are good; the average absolute discrepancy for the two systems is only 0·2 per cent. The theoretically calculated values of D_{12} for Kr–C_2H_5Cl system using the force constant for ethyl chloride from viscosity [8] are in fair agreement with the observed values. the average discrepancy is about 0·7 per cent. But for Kr–CH_2Cl_2 system the agreement is less good. The D_{12} values calculated by using the force constants for CH_2Cl_2 from viscosity [8] overestimates the experimental values by about 3·2 per cent.

It is interesting to note that the theoretically calculated values of D_{12} using the force constants for polar gas from $B(T)$ data are much larger than the experimental D_{12} values for Kr–CH_2Cl_2 system like other polar–nonpolar mixtures studied by Srivastava and Saran [6, 7] but for Kr–C_2H_5Cl, they are much lower, the higher value of D_{12} comes probably due to the fact that the value of σ for CH_2Cl_2 as obtained from $B(T)$ data on Stockmayer potential are much smaller than those obtained from viscosity. By applying the off-centre model of Blanks and Prausnitz [2] Srivastava and Saran [6, 7] have shown that the virial data of polar gases also give reasonable parameters for unlike interactions. Due to the non-availability of reliable critical data of CH_2Cl_2 in literature, we have not applied the off-centre model for it. But for C_2H_5Cl, the collision diameter $\sigma_{jj(np)}$ due to nonpolar forces approximated from,

$$\sigma_{jj(np)} = 0{\cdot}94\,(V_{c_j})^{\frac{1}{3}} \tag{9}$$

in which V_{c_j} is the critical volume in cm^3/mol, is less (= 4·875 Å) than that obtained from second virial data on the Stockmayer model (= 5·41 Å). According to Blanks and Prausnitz [2] the correction factor K_j which comes in combination rules through;

$$\xi_{ij} = \frac{K_j\alpha_i\mu_j^2}{4\left[\dfrac{\sigma_{ii}+\sigma_{jj(np)}}{2}\right]^6(\epsilon_{ii}\epsilon_{jj(np)})^{\frac{1}{2}}} \tag{10}$$

where

$$\epsilon_{jj(np)} = \beta\frac{\alpha_j^2 I_j}{\sigma_{jj(np)}^6}. \tag{11}$$

I_j is ionization potential and proportionality constant β is equal to 4·82 × 10^3 °K/eV, is due to the off-centre dipole and is equal to unity for ideal dipole situated at the centre of the molecule and for all other cases greater than unity. Their plot of K_j against $(\sigma_{jj(np)} - \sigma_{\text{Stockmayer}})/\sigma_{jj(np)}$ takes account of only those gases for which the latter is positive. But for C_2H_5Cl it is found that $(\sigma_{jj(np)} - \sigma_{\text{Stockmayer}})/\sigma_{jj(np)}$ is about $-0{\cdot}11$ and if the plot is extrapolated for negative values then K_j comes equal to 0·35. The force parameters thus obtained [from (3) to (5) and (9) to (11)] are recorded in column 6 of Table 2 and D_{12} values calculated from these force parameters are given under column (d) of Table 1. The agreement with experimental D_{12} values is not good but better than that obtained with the force parameters obtained from second virial data on Stockmayer potential. Probably one of the reasons for this discrepancy is that equation (11) does not hold good for C_2H_5Cl due to its nonsphericity. The conclusion of Blanks and Prausnitz that the value of K_j must not be less than unity, may not be true in view of the recent experiments [16] where it has been concluded that certain molecules may prefer repulsive dipole–dipole orientations. For repulsive orientation, the correction term to the induction energy due to off-centre nature of dipole will be negative and thus K_j will be less than unity.

Recently Storvick and Mason [17] have developed a method of finding out D_{12} value from the viscosity data of binary mixtures. However, no viscosity data are available for either of the binary mixtures considered here.

REFERENCES

1. J. O. HIRSCHFELDER, C. F. CURTISS and R. B. BIRD, *Molecular Theory of Gases and Liquids.* John Wiley, New York (1954).
2. R. F. BLANKS and J. M. PRAUSNITZ, Volumetric properties of gas mixtures containing one or more polar components, *A.I.Ch.E. Jl* **8**, 86–92 (1962).
3. B. N. SRIVASTAVA and I. B. SRIVASTAVA, Studies on mutual diffusion of polar–nonpolar gas mixtures, *J. Chem. Phys.* **36**, 2616–2620 (1962).
4. I. B. SRIVASTAVA, Mutual diffusion of binary mixtures of ammonia with He, Ne and Xe, *Ind. J. Pure Appl. Phys.* **36**, 193–199 (1962).
5. A. SARAN and Y. SINGH, Multicomponent diffusion in the ^{85}Kr–SO$_2$–Kr system, *Can. J. Chem. Engng* **44**, 2222–2223 (1966).
6. B. N. SRIVASTAVA and A. SARAN, Mutual diffusion studies in krypton–acetone and krypton–chloroform systems, *Physica, 's Grav.* **32**, 110–118 (1965).
7. B. N. SRIVASTAVA and A. SARAN, Mutual diffusion in polar–nonpolar gases: krypton–sulphur dioxide and krypton–diethyl ether, *Can. J. Phys.* **44**, 2595–2600 (1966).
8. L. MONCHICK and E. A. MASON, Transport properties of polar gases, *J. Chem. Phys.* **35**, 1676–1697 (1961).
9. J. S. ROWLINSON, The second virial coefficients of polar gases, *Trans. Faraday Soc.* **45**, 974–984 (1949).
10. E. P. NEY and F. C. ARMISTEAD, The self-diffusion coefficient of uranium hexafluoride, *Phys. Rev.* **71**, 14–19 (1947).
11. B. N. SRIVASTAVA and R. PAUL, Multicomponent diffusion in the system ^{85}Kr-, *Physica, 's Grav.* **28**, 646–652 (1962).
12. B. N. SRIVASTAVA and I. B. SRIVASTAVA, Mutual diffusion coefficient of the polar gases; ammonia and diethyl ether, *J. Chem. Phys.* **38**, 1183–1186 (1962).
13. D. G. CLIFTON, Measurement of viscosity of krypton, *J. Chem. Phys.* **38**, 1123–1131 (1962).
14. B. E. F. FENDER and G. D. HALSEY, JR. Second virial coefficients of Argon, Krypton, and Argon–Krypton mixtures at low temperatures. *J. Chem. Phys.* **36**, 1881–1888 (1962).
15. A. PEREZ MASIÁ and M. DIAZ PEÑA, The second virial coefficient of organic vapours. I. Experimental results, *An. R. Soc. Esp. Fis. Quim.* **54B**, 661–668 (1958).
16. A. K. PAUL and A. K. BARUA, Intermolecular potentials and viscosities of some polar organic vapours. *Br. J. Appl. Phys.*, to be published.
17. T. S. STORWICK and E. A. MASON, Determination of diffusion coefficients from viscosity measurements; effects of higher Chapman–Enskog approximation, *J. Chem. Phys.* **45**, 3752–3754 (1966).

Résumé—Les coefficients de diffusion binaires de gaz ayant un composant polaire ont été mesurés dans la gamme de température 275 à 318°K en employant la technique des deux réservoirs de Ney et Armistead. Les systèmes étudiés étaient *Kr*—CH_2Cl_2 et *Kr*—C_2H_5Cl. Le krypton radioactif ^{85}Kr a été employé comme traceur et un compteur à scintillation déterminait sa concentration à différents instants. La corrélation de masse a été appliquée pour obtenir les coefficients normaux de diffusion pour les deux systèmes.

Les valeurs expérimentales de D_{12} ont été employées pour obtenir les paramètres d'interaction différente du potentiel de Lennard-Jones (12 : 6) et comparées avec celles obtenues en utilisant les règles de combinaison pour un système polaire-non polaire et les constantes de force du gaz polaire à partir de la viscosité aussi bien qu'a partir des données du second viriel. Le modèle décentré de Blanks et Prausnitz est discuté en détail.

Zusammenfassung—Binäre Diffusionskoeffizienten von Gasen mit einem polaren Bestandteil wurden im Temperaturbereich von 275 bis 318°K gemessen mit Hilfe der zwei-Kugel Technik von Ney und Armistead. Die untersuchten Systeme waren Kr—Ch_2Cl_2 und Kr—C_2H_5Cl. Radioaktives ^{85}Kr wurde als Spurmaterial verwendet, und ein Szintillationszähler diente zur Konzentrationsbestimmung zu verschiedenen Zeiten. Mit Hilfe der Massenkorrektur war es möglich die normalen Diffusionskoeffizienten für beide Systeme zu erhalten.

Die experimentallen D_{12} Werte dienten dazu, die ungleichen Reaktionsparameter für das Lennard-Jones (12:6) Potential zu erhalten und sie wurden mit jenen verglichen, die unter Benutzung der Kombinationsgesetze für ein polares-nichtpolares System und der Kraftkonstanten eines polaren Gases aus der Zähigkeit wie auch aus den zweiten Virialwerten erhalten wurden. Das "Ausser-Mitte" Modell von Blanks und Prausnitz wurde im einzelnen diskutiert.

Аннотация—С помощью методики Нея и Армистеда измерены коэффициенты бинарной диффузии газов с одной полярной составляющей в интервале температур 275°–318°K. Исследовались системы Kr—Ch_2Cl_2 и Kr—C_2H_5Cl. В качестве изотопного индикатора использовался радиоактивный ^{85}Kr, концентрация которого в различные промежутки времени определялась сцинтилляционным счётчиком. Для получения нормальных коэффициентов диффузии обеих систем вводилась массовая поправка.

С помощью экспериментальных значений D_{12} определялись параметры взаимодействия потенциала Леннарда-Джонса (12:6) и производилось сравнение со значениями, полученными с помощью комбинационных правил для полярной-неполярной системы, и с силовыми постоянными полярного газа, полученными из значений вязкости, а также из значения второго вириального коэффициента. Подробно рассмотрена нецентрированная модель Блэнкса и Праусница.