Table VI. Values of the Parameters in the McAllister Three-Body Model

system	$\nu_{AB} \times 10^6$, m^2/s	$\nu_{BA} \times 10^6$, m^2/s	std dev, m^2/s
n-hexane (A)–*n*-heptane (B)	0.51	0.56	1.2×10^{-10}
n-hexane (A)–*n*-octane (B)	0.57	0.67	2.7×10^{-10}
n-hexane (A)–*n*-decane (B)	0.72	0.96	5.9×10^{-10}
n-heptane (A)–*n*-octane (B)	0.66	0.71	2.0×10^{-10}
n-heptane (A)–*n*-decane (B)	0.80	1.02	4.4×10^{-10}
n-heptane (A)–*n*-dodecane (B)	1.01	1.44	1.1×10^{-9}
n-heptane (A)–*n*-tetradecane (B)	1.30	2.02	3.6×10^{-9}
n-octane (A)–*n*-decane (B)	0.93	1.08	6.3×10^{-10}
n-octane (A)–*n*-tetradecane (B)	1.42	2.12	2.5×10^{-9}
n-tetradecane (A)–*n*-hexadecane (B)	3.47	3.94	2.0×10^{-9}

behavior than the rest of the systems reported in this study.

The experimental kinematic viscosity–composition data were fitted to the McAllister three-body model given by the following equation:

$$\ln \nu_m = X_A^3 \ln \nu_A + 3X_A^2X_B \ln \nu_{AB} + 3X_AX_B^2 \ln \nu_{BA} + X_B^3 \ln \nu_B - \ln\left[X_A + X_B\frac{M_B}{M_A}\right] + 3X_A^2X_B \times \ln\left[\left[2 + \frac{M_B}{M_A}\right]/3\right] + 3X_AX_B^2 \ln\left[\left[1 + 2\frac{M_B}{M_A}\right]/3\right] + X_B^3 \ln\left[\frac{M_B}{M_A}\right] \quad (5)$$

where ν_{AB} and ν_{BA} are adjustable parameters that can be obtained from experimental data. Table VI lists the values of the parameters ν_{AB} and ν_{BA} for the systems investigated in this study. The standard deviation of the fit indicates that the model given by eq 5 fits the experimental data very well.

Conclusions

The densities and kinematic viscosities of 10 *n*-alkane binary mixtures have been determined at 293.15 K. The reproducibility of determining the density and kinematic viscosity data is 2×10^{-5} kg/L and 6×10^{-10} m²/s, respectively.

If the additivity of volumes on mixing is employed as a criterion of ideal solution behavior, then all the systems reported herein, with the exception of the systems *n*-hexane–*n*-decane and *n*-heptane–*n*-tetradecane, approach ideal behavior.

The experimental data were correlated by using polynomial expressions that fitted the data well. Also, the McAllister three-body model gave an excellent fit to the experimental kinematic viscosity–composition data.

Nomenclature

A	adjustable parameter
B	adjustable parameter
C_1	calibration constant
C_2	calibration constant
E	calibration constant
X	mole fraction
ν	kinematic viscosity
ρ	density
ω	mass fraction

Subscripts

A	first-named component in a binary mixture
m	mixture

Registry No. *n*-Hexane, 110-54-3; *n*-heptane, 142-82-5; *n*-octane, 111-65-9; *n*-decane, 124-18-5; *n*-dodecane, 112-40-5; *n*-tetradecane, 629-59-4; *n*-hexadecane, 544-76-3.

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Received for review June 25, 1990. Accepted November 26, 1990. We acknowledge with thanks financial support from the Natural Sciences and Engineering Research Council of Canada (NSERC).

Excess Enthalpy of Binary Systems of Halothane + Cyclic Ethers

Romolo Francesconi*

Dipartimento di Chimica "G. Ciamician", Università degli Studi, via Selmi 2, 40126 Bologna, Italy

Fabio Comelli

Centro di Studio per la Fisica delle Macromolecole del CNR, via Selmi 2, 40126 Bologna, Italy

The excess molar enthalpies H^E of binary liquid systems of halothane + cyclic ethers (1,4-dioxane, oxane, or oxolane) were determined at atmospheric pressure and 298.15 K by using an isothermal flow microcalorimeter. The experimental data were correlated by means of the Redlich–Kister equation. The systems are highly exothermic, $H^E < 0$, with asymmetric H^E vs composition curves.

Introduction

This work pursues our systematic studies on the excess molar enthalpies H^E of binary systems containing halothane (2-bromo-2-chloro-1,1,1-trifluoroethane) with cyclic ethers with the aim of investigating the influence of the oxygen atoms on the properties of ether + halothane mixtures. In a previous paper (*1*), the binary system halothane + 1,3-dioxolane has

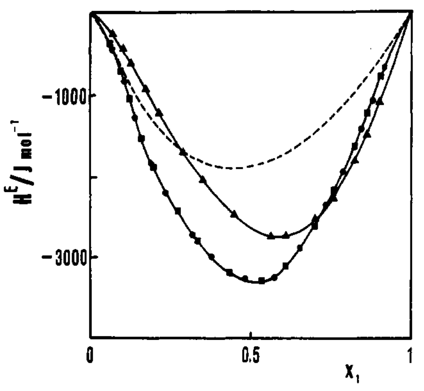

Figure 1. Excess molar enthalpy H^E for halothane (1) + ethers (2) at 298.15 K, as a function of the mole fraction x_1 of halothane: --, 1,3-dioxolane (*1*); ▲, 1,4-dioxane; ●, oxane; ■, oxolane; —, result calculated by eq 1 with parameters a_k of Table I.

been studied. The cyclic ethers used at present are 1,4-dioxane, oxane, and oxolane.

Experimental Section

Materials. All materials were Aldrich products, with the exception of oxane, which was from Fluka. Halothane (analytical grade, 99%, stabilized with 0.01% thymol) was purified as described in ref 1. 1,3-Dioxolane, oxane, oxolane, and 1,4-dioxane were the same as those specified in ref 2. Before the actual measurements, all the solvents were stored in the dark over molecular sieves (Union Carbide type 4A, $^1/_{16}$-in. pellets).

***Density* Measurements.** The densities ρ of the pure components, necessary to determine fluxes in calorimetric measurements, have been reported in our previous papers (*1*–*3*).

Calorimetric Measurements. The excess molar enthalpies H^E were determined at 298.15 ± 0.05 K at atmospheric pressure as a function of the mole fraction x_1 of halothane by using a flow microcalorimeter Model 2107, LKB Produckter AB (Bromma, Sweden), described in ref 4, reporting also details on electrical calibration and analytical measurements. The performance of the microcalorimeter was checked by measuring H^E of the test mixture cyclohexane + hexane (*5*), and the agreement with literature data was within 0.5% in the central range of x_1.

The estimated accuracy of the calorimetric data is about 1%. The experimental H^E data are listed in Table I and presented graphically in Figure 1.

The H^E values were fitted to the Redlich–Kister equation

$$H^E_{\text{calc}}/(\text{J mol}^{-1}) = x_1 x_2 \sum_{k\geq 0} a_k (x_1 - x_2)^k \qquad (1)$$

by the method of least-squares (*3*). The adjustable parameters a_k and the standard deviations

$$\sigma(H^E) = [\sum(H^E - H^E_{\text{calc}})/(N - n)]^{0.5} \qquad (2)$$

where N is the number of experimental points and n the number of coefficients a_k, are listed in Table I.

Table I. Experimental Excess Molar Enthalpies H^E for the Halothane (1) + Ether (2) Systems as a Function of the Mole Fraction x_1 of the Halothane at 298.15 K, Coefficients a_k, Equation 1, and Standard Deviations $\sigma(H^E)$, Equation 2

	1,4-dioxane		oxane		oxolane	
	x_1	H^E/(J mol^{-1})	x_1	H^E/(J mol^{-1})	x_1	H^E/(J mol^{-1})
	0.0629	−268	0.0714	−403	0.0604	−414
	0.0915	−432	0.1034	−831	0.0875	−717
	0.1184	−604	0.1331	−1238	0.1133	−1038
	0.1677	−919	0.1874	−1854	0.1609	−1505
	0.2118	−1206	0.2352	−2234	0.2036	−1900
	0.2872	−1689	0.3157	−2764	0.2772	−2428
	0.3495	−2043	0.3809	−3006	0.3383	−2808
	0.4463	−2495	0.4799	−3276	0.4340	−3226
	0.5606	−2755	0.5806	−3177	0.5349	−3294
	0.6171	−2741	0.6486	−2885	0.6053	−3103
	0.7074	−2508	0.7346	−2338	0.6970	−2623
	0.7633	−2254	0.7868	−1926	0.7541	−2179
	0.8287	−1801	0.8470	−1406	0.8215	−1608
	0.8658	−1452	0.8807	−1057	0.8599	−1222
	0.9063	−1070	0.9172	−669	0.9020	−799
a_0	−10648		−13151		−13287	
a_1	−4569		−429		−563	
a_2	2478		6479		8215	
a_3			7525		3992	
a_4			−17664		−15972	
a_5			−11831		−3964	
a_6			27107		19873	
$\sigma(H^E)^a$	12		14		14	

^{a} Units for $\sigma(H^E)$: J mol^{-1}.

Conclusions

As can be seen from Figure 1, all the systems show large negative excess molar enthalpies H^E with strongly asymmetric H^E vs x_1 curves. This common feature can be ascribed to the strong interactions (probably of hydrogen bond type) between the positively charged H atom of halothane and the negatively charged O atoms of ethers.

Glossary

a_k	parameters in eq 1
H^E	excess molar enthalpy, J mol^{-1}
x_i	mol fraction of component i (i = 1, halothane; i = 2, ethers)

Greek Symbols

$\sigma(H^E)$	standard deviation, eq 2, J mol^{-1}

Registry No. 1,4-Dioxane, 123-91-1; oxane, 142-68-7; oxolane, 109-99-9; halothane, 151-67-7.

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Received for review June 27, 1990. Accepted March 5, 1991. This work is partly supported by CNR, Roma, Italy "Progetto Finalizzato Chimica Fine II".