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Excess molar enthalpies of ternary and constituent binary systems {1,2-dichloropropane+2-propanol+2-butanol} at T=298.15 K

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Abstract−Ternary excess molar enthalpies at T=298.15 K and P=101.3 kPa for the system of {1,2-dichloropropane+2-propanol+2-butanol} and their constituent binary systems {1,2-DCP+2-propanol}, {1,2-DCP+2-butanol}, and {2-propanol+2-butanol} have been measured over the whole composition range using an isothermal micro-calorimeter with flow-mixing cell. All of the binary and ternary systems, including three pseudobinary systems, show endothermic behavior except for the binary mixture {2-propanol+2-butanol}, which shows small exothermicity. The Redlich-Kister equation was used to correlate the binary $H^{E}_{m,ij}$ data, and the Morris equation to correlate the ternary $H^{E}_{m,123}$ data. Comparisons between the Morris and Radojkovič equations for the prediction of $H^{E}_{m,123}$ have been also made. The experimental results have been qualitatively discussed in terms of self-association, isomeric effect and chain length among molecules.

Key words: Excess Molar Enthalpy, Ternary System, Binary Systems, 1,2-Dichloropropane, 2-Propanol, 2-Butanol

INTRODUCTION

Thermo-physical properties are beneficial for characterizing the type and magnitude of molecular interaction in these binary and ternary mixtures, giving important information in many practical problems concerning process design and simulation. In addition, knowledge of these excess molar properties can be useful in predicting the solution behavior of mixtures. In recent years, a number of attempts have been made to provide reliable excess properties of binary mixtures; however, experimental data for ternary mixtures remain quite scarce.

As a continuation of our experimental studies on the excess properties of 1,2-dichloropropane (1,2-DCP) with various non-electrolytes [1-7], this project was undertaken to measure the excess molar enthalpies at T=298.15 K for the ternary mixture {1,2-DCP+2-propanol+2-butanol} and for the constituent binary mixtures {1,2-DCP+2-propanol}, {1,2-DCP+2-butanol} and {2-propanol+2-butanol}. No literature data on H^{E}_{m} at T=298.15 K were found for these ternary and binary systems.

In a previous study, we determined the excess properties of the binary systems for 1,2-DCP with 1-alkanols [4] at T=298.15 K; the effect on H^{E}_{m} due to chain length as well as intermolecular forces has been discussed. The binary excess enthalpy data were fitted to the Redlich-Kister [8] equation. Several expressions to predict excess enthalpy for the ternary system are available in the literature. Here, the Morris model [9] was used to correlate the experimental ternary excess enthalpy data. The predictions by different methods with experimental values of the excess properties were compared.

EXPERIMENTAL SECTION

1. Materials

1,2-DCP (Fluka, Switzerland, >99%), 2-propanol and 2-butanol (Signa-Aldrich, USA, >99.5% for both chemicals) were used without further purification but degassed by means of an ultrasonic bath. The stated purities of the chemicals were checked by gas chromatographic analysis. HPLC grade water (Fisher Scientific, >99.7%) was used for calibration of the refractometer and densimeter. The purity of the chemicals was also checked by measuring and comparing the refractive indices and densities at T=298.15 K and atmosphere pressure with their corresponding literature values [10,11] as shown in Table 1. These results of pure components are in good agreement with literature data. Refractive indices were measured using a refractometer (model RA-520, Kyoto Electronics, Japan) with a resolution of ±2×10^{-5} for values ranging from 1.32 to 1.58 and a precision of ±0.01 K. The densities of pure components and their corresponding binary mixtures {x (2-propanol)+(1−x) 2-buta-

Table 1. Densities ρ, refractive indices n^{25}_{D}, and purities of chemicals for pure components at T=298.15 K

Compound	ρ [g/cm^3]		n^{25}_{D}		GC analysis [mass%]
	Exptl.	Lit.[a]	Exptl.	Lit.[a]	
1,2-DCP	1.14912	1.14936	1.43668	1.43679	99.0
2-Propanol	0.78081	0.78126 0.7807[b]	1.37506	1.3752	99.6
2-Butanol	0.80234	0.80241	1.39523	1.3953	99.6

[a] Ref. [10]
[b] Ref. [11]

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nol} having a fixed molar ratio x/(1−x)≈0.3, 1.0 and 3.0 were measured by a vibrating-tube densimeter (model DMA 58, Anton Paar, Graz, Austria) at T=298.15 K with an accuracy $\pm1\times10^{-5}$ g/cm^3 and a precision of sample thermometer of ±0.01 K.

2. Apparatus and Procedure

The experimental excess molar enthalpies were measured with an isothermal microcalorimeter (model CSC-4400, Calorimetry Sciences Corporation, Utah, U.S.A) equipped with a newly designed flow-mixing assembly kit (model CSC-4442, CSC, Utah, U.S.A). The pseudobinary mixtures were prepared by mass using an electronic balance with a precision of $\pm1.5\times10^{-5}$ g (model AT-201, Mettler Toledo, Switzerland). Two ISCO high precision, positive displacement, syringe-type pumps (model 500D, Teledyne Isco Inc.) were used to establish constant flow rates through the mixing cell. Each pump (of variable flow rate from 0.001 to 138 cm^3/min) was calibrated by determining the volumetric flow rates from 0.001 cm^3/min to 1.0 cm^3/min of bi-distilled water, and empirical correction equations were fitted for each pump. Pump calibrations were linear and indicated a reliability of better than ±0.7% of the set flow rate (the flow accuracy stated is ±0.5% of setpoint) over the entire calibrated range. Working pressure of the mixing cell in the calorimeter was controlled at P=101.3 kPa by a back-pressure regulator (Grove Valves & Regulator Co., Stafford, TX, U.S.A).

Prior to this study, performance testing was again done due to newly equipped ISCO syringe pumps connected to the measuring apparatus of calorimeter with the systems {cyclohexane+n-hexane at T=298.15 K} (endothermic effect) and {water+ethanol at T=298.15 K} (exothermic effect) recommended as reference mixtures in isothermal calorimeters [12,13]. The pre-experimental results were compared with the results of Tanaka et al. [14], Christensen et al. [15] and Ott et al. [16] for the system {cyclohexane+n-hexane}, and Chand and Fenby [17] and Costigan et al. [18] for the system {water+ethanol} in Figs. 1 and 2, respectively. As can be seen from these figures, the experimental excess enthalpy values measured by a microcalorimeter with newly equipped pumps were well in agreement with the literature values. The results were found to differ by less than 0.6% from those of Tanaka et al., Christensen et al. and Otto et al. However, when the results focused on the system {water+ethanol}, the differences among those experimental values were to some extent larger than those of the system {cyclohexane+n-hexane}. Details of an isothermal flow calorimeter, calibrations of calorimeter and experimental procedure, including the determination of baseline values of heat flux to obtain excess enthalpies, have been described in previous work [1-3,19]. In this study, the total volumetric flow rate was 0.1 cm^3/min, depending on the magnitude of the measured heat signal. The uncertainty in excess molar enthalpy measurement was estimated to be better than ±1.0%. Similarly, the uncertainty of the mole fraction was estimated to be less than $\pm1\times10^{-3}$.

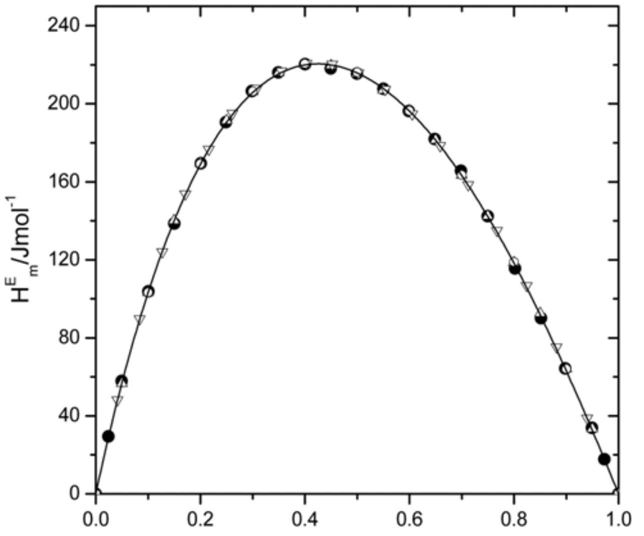

Fig. 1. Comparisons of the experimental results for {x_1 C_6H_{12}+x_2 C_6H_{14}} with literature values at 298.15 K: △, Tanaka et al. [14]; ▽, Christensen et al. [15]; ○, Ott et al. [16]; ●, this work. Solid line: calculated using Redlich-Kister equation.

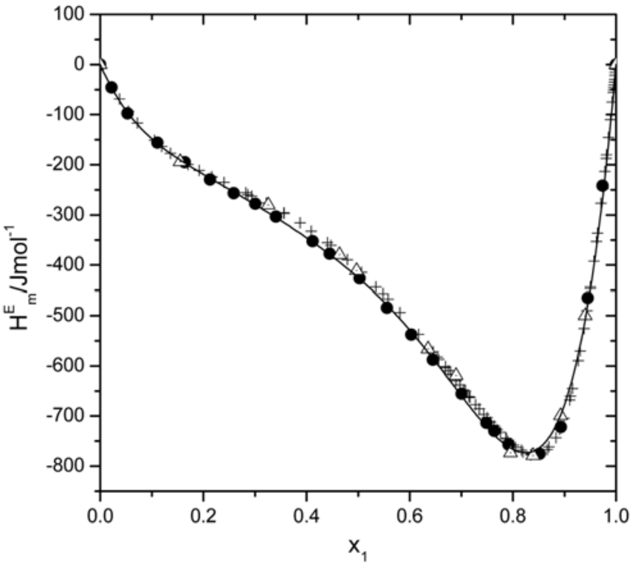

Fig. 2. Comparisons of the experimental results for {x_1 H_2O+x_2 C_2H_5OH} with literature values at T=298.15 K: △, Chand and Fenby [17]; +, Costigan et al. [18]; ●, this work. Solid line: calculated using Redlich-Kister equation.

Each experimental run for the measurement of the ternary excess molar enthalpies was performed by adding one component to a binary mixture of the other two. A ternary mixture is regarded as a pseudobinary system made up of one binary mixture and the third component.

In this ternary system, one mole of the ternary mixture was prepared by mixing $(1-x_1)$ of the binary mixture composed of {x_1'2-propanol (2)+x_2'2-butanol (3)}, where $x_2'=1-x_1'$, and x_1 of 1,2-DCP (1). For this purpose binaries with fixed molar ratios $x_1'/x_2'\approx0.3$, 1.0 and 3.0, were prepared by mass. The ternary excess molar enthalpy $H^E_{m,123}$ at the pseudobinary composition x_1, x_2, and $x_3(=1-x_1-x_2)$ was then obtained according to the following relation:

$$H^E_{m,123}=H^E_{m,1+23}+(1-x_1)H^E_{m,23} \qquad (1)$$

where x_1 is the mole fraction of the component 1 (1,2-DCP) in the ternary mixture, and the $H^E_{m,1+23}$ is experimental excess enthalpy for pseudobinary mixtures and $H^E_{m,23}$ is the excess molar enthalpy

Table 2. Experimental excess molar enthalpies $H^E_{m,jk}$ for binary mixtures {x (1,2-DCP)+(1−x) 2-propanol}, {x (1,2-DCP) +(1−x) 2-butanol} and {x (2-propanol)+(1−x) 2-butanol} at T=298.15 K

x	$H^E_{m,jk}$ (J/mol)	x	$H^E_{m,jk}$ (J/mol)
	x (1,2-DCP)+(1−x) 2-propanol		
0.021	88.0	0.550	1474.1
0.053	255.0	0.603	1485.5
0.103	455.8	0.646	1478.9
0.153	635.5	0.702	1429.7
0.196	814.8	0.747	1360.4
0.250	976.7	0.805	1223.5
0.304	1133.0	0.853	1064.1
0.351	1241.3	0.901	857.2
0.399	1338.0	0.951	538.6
0.448	1410.1	0.976	308.7
0.498	1457.2		
	x (1,2-DCP)+(1−x) 2-butanol		
0.025	184.3	0.554	1871.5
0.054	372.7	0.605	1864.0
0.101	635.3	0.646	1820.3
0.149	933.1	0.697	1751.5
0.198	1139.7	0.749	1645.1
0.246	1331.9	0.801	1483.6
0.295	1515.7	0.853	1259.8
0.354	1671.3	0.895	1012.9
0.404	1754.4	0.948	604.9
0.453	1830.6	0.970	396.8
0.504	1854.2		
	x (2-propanol)+(1−x) 2-butanol		
0.022	−1.6	0.546	−13.7
0.046	−3.0	0.606	−12.6
0.093	−5.6	0.654	−11.7
0.151	−8.5	0.701	−10.7
0.197	−10.4	0.748	−9.5
0.252	−12.0	0.803	−7.6
0.296	−12.9	0.856	−5.7
0.350	−13.9	0.900	−4.1
0.403	−14.1	0.952	−2.1
0.455	−14.4	0.978	−1.0
0.496	−14.2		

of the binary mixtures composed of components 2 (2-propanol) and 3 (2-butanol). Values of $H^E_{m,23}$ at three different mole fractions were obtained by Eq. (2) using parameters listed in Table 3. Eq. (1) does not involve any approximation.

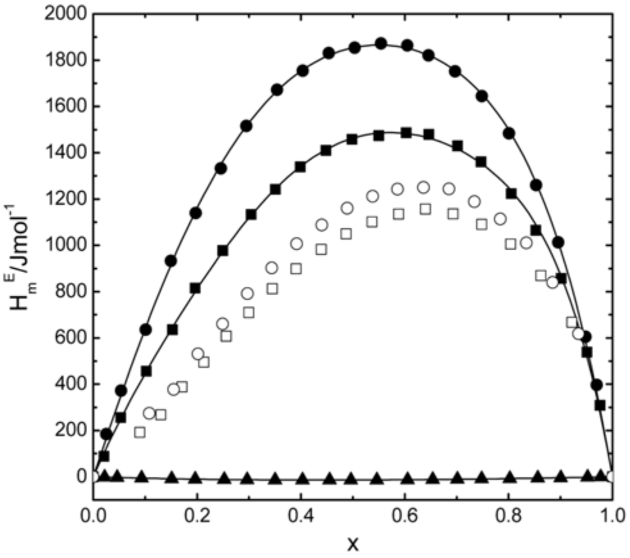

Fig. 3. Excess molar enthalpies, $H^E_{m,jk}$ (J/mol) of binary mixtures at T=298.15 K and atmospheric pressure. Experimental results: (■, $H^E_{m,12}$), x (1,2-DCP)+(1−x) 2-propanol; (●, $H^E_{m,13}$), x (1,2-DCP)+(1−x) 2-butanol; (▲, $H^E_{m,23}$), x (2-propanol)+ (1−x) 2-butanol. Solid lines: calculated with Eq. (2) using parameters listed in Table 3. Previously reported results: □, x (1,2-DCP)+(1−x) 1-propanol; ○, x (1,2-DCP)+(1−x) 1-butanol.

RESULTS AND DISCUSSION

The experimental excess molar enthalpies $H^E_{m,ij}$ (i<j), for the constituent three binary mixtures of {1,2-DCP (1)+2-propanol (2)}, {1,2-DCP (1)+2-butanol (3)} and {2-propanol (2)+2-butanol (3)} at T=298.15 K and atmospheric pressure, are listed in Table 2 and the results are also reported graphically in Fig. 3.

The composition dependence of the experimental excess molar enthalpies $H^E_{m,ij}$ of binary mixtures has been described by the following Redlich-Kister [8] equation:

$$H^E_{m,ij}(\text{J/mol}) = x_i(1-x_i)\sum_{p=1}^{n} A_p(2x_i-1)^{p-1} \qquad (2)$$

where x_i is the mole fraction of the first component in the binary mixture and n is the number of parameters. A_p are the adjustable parameters determined by minimizing the sum of squares of the differences between experimental values of $H^E_{m,ij}$ and the corresponding values calculated by Eq. (2) using a non-linear regression procedure. The optimal number of the parameters, A_p, was determined by applying an *F*-test [20] with an examination of the variation of the standard deviation σ:

Table 3. Adjustable parameters A_i of Redlich-Kister equation in Eq. (2) with standard deviation σ (J/mol) for constituent binary systems at T=298.15 K

Binary systems	A_1	A_2	A_3	A_4	A_5	σ (J/mol)
x (1,2-DCP)+(1−x) 2-propanol	5852.5	1380.5	784.7	2478.4	2365.9	15.3
x (1,2-DCP)+(1−x) 2-butanol	7414.4	956.5	2498.8	2240.7		14.9
x (2-propanol)+(1−x) 2-butanol	−56.5	14.1				0.09

Table 4. Experimental excess molar enthalpies, $H^E_{m,123}$ for the ternary mixture $\{x_1$ (1,2-DCP)$+x_2$ (2-propanol)$+(1-x_1-x_2)$ 2-butanol$\}$ at T=298.15 K and atmospheric pressure

x_1	x_2	$H^E_{m,1+23}$ (J/mol)	$H^E_{m,123}$ (J/mol)	x_1	x_2	$H^E_{m,1+23}$ (J/mol)	$H^E_{m,123}$ (J/mol)
			$x'_1/x'_2=0.3247$, $H^E_{m,23}$ (J/mol)$=-11.8$				
0.098	0.221	587.3	577.1	0.595	0.099	1796.5	1792.4
0.200	0.196	1066.0	1057.4	0.699	0.074	1699.6	1696.5
0.296	0.173	1403.0	1395.7	0.805	0.048	1427.2	1425.1
0.403	0.146	1672.5	1665.5	0.902	0.024	959.6	958.5
0.503	0.122	1793.2	1788.2				
			$x'_1/x'_2=0.9996$, $H^E_{m,23}$ (J/mol)$=-14.1$				
0.094	0.453	527.6	511.4	0.595	0.203	1708.6	1700.9
0.194	0.403	983.7	968.3	0.700	0.150	1612.6	1605.0
0.297	0.352	1313.3	1296.8	0.798	0.101	1401.0	1396.1
0.403	0.299	1527.4	1512.5	0.898	0.051	944.2	942.0
0.503	0.249	1671.0	1658.0				
			$x'_1/x'_2=2.9973$, $H^E_{m,23}$ (J/mol)$=-9.3$				
0.098	0.677	489.5	484.2	0.601	0.299	1600.6	1601.4
0.202	0.598	922.8	918.8	0.698	0.226	1498.8	1499.2
0.303	0.523	1245.0	1242.2	0.799	0.150	1290.6	1290.6
0.398	0.451	1451.3	1451.9	0.905	0.072	857.4	857.1
0.498	0.377	1578.6	1579.5				

$$\sigma=\left[\frac{\sum_{l=1}^{N}(H^E_{m,ij(exp)}-H^E_{m,ij(calc)})_l^2}{N-n}\right]^{1/2} \tag{3}$$

where N is the number of experimental points and n is the number of adjustable parameters. All the parameters of Eq. (2) are reported in Table 3 together with the standard deviations σ of the fits.

As shown in Fig. 3, the excess molar enthalpies $H^E_{m,ij}$ for the binary mixtures $\{x$ (1,2-DCP) (1)$+(1-x)$ 2-propanol (2)$\}$ and $\{x$ (1,2-DCP) (1)$+(1-x)$ 2-butanol (3)$\}$ are positive, while the binary mixture $\{x$ (2-propanol) (2)$+(1-x)$ 2-butanol (3)$\}$ are slightly negative over the whole range of composition. To help understand the trends of experimental $H^E_{m,ij}$ values between 2-alkanols and 1-alkanols with 1,2-DCP, the previously reported results [4] are also presented in Fig. 3.

The $H^E_{m,ij}$ values reported are mainly considered as two contributions of opposite effects: (i) an endothermic effect (positive values) due to the disruption of the associated hydrogen bonding in 2-alkanols for {1,2-DCP+2-propanol} and {1,2-DCP+2-butanol}, and (ii) an exothermic effect (negative values) due to the formation of hydrogen-bonded complexes between unlike 2-alkanol molecules for {2-propanol+2-butanol}. In the case of the mixtures for {1,2-DCP+2-propanol, and +2-butanol}, effect (i) is consistent with our previous work [4]. From the results of this work it can be observed that as the chain length of 2-alkanols increases in length, the mixture becomes more endothermic, even though they do not have much difference in polarity.

Combining the results of this work and our previous work [4], the isomeric effects for the binary mixtures 1,2-DCP with 1-, and 2-propanols and 1-, and 2-butanol can be also examined. For a given mixtures with isomers of 1- and 2-alkanols the maximum H^E_m values increase in the sequence, respectively: 1-propanol<2-propanol, and 1-butanol<2-butanol. Comparing these results with Lafuente et al. [21], a similar trend was found in both cases.

The experimental excess enthalpy $H^E_{m,1+23}$ for the pseudobinary mixtures and the corresponding values of $H^E_{m,123}$, calculated from Eq. (1), for the ternary system $\{x_1$ 1,2-dichloropropane$+x_2$ 2-propanol $+x_3$ 2-butanol$\}$ at T=298.15 K are listed in Table 4. The values of $H^E_{m,1+23}$ are plotted in Fig. 4, along with curves of the constituent binary systems for comparison. The $H^E_{m,1+23}$ values indicate that the prevailing effect is the disruption of the association due to hydro-

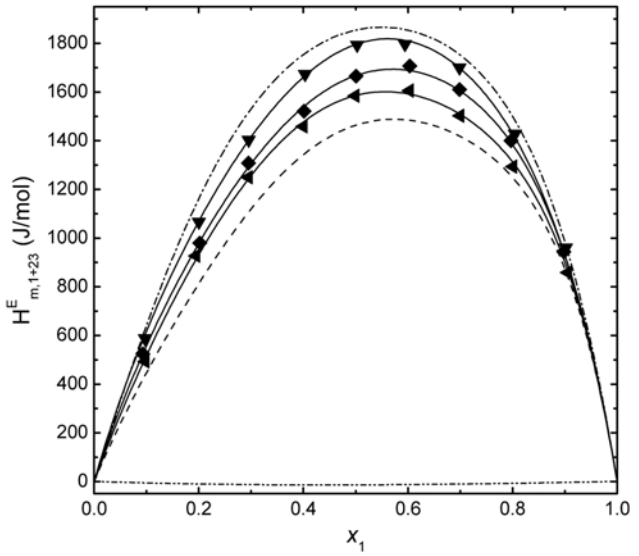

Fig. 4. Excess molar enthalpies, $H^E_{m,1+23}$ for the ternary mixture $\{x_1$ (1,2-DCP)$+x_2$ (2-propanol)$+x_3$ (2-butanol)$\}$ at T=298.15 K and atmospheric pressure. Experimental results: (▼), $x'_1/x'_2=0.3247$; (◆), $x'_1/x'_2=0.9996$; (◀), $x'_1/x'_2=2.9973$. Solid lines: calculated using Redlich-Kister equation. Dotted lines: (–·–), x_1 (1,2-DCP)$+(1-x_1)$ 2-butanol; (---), x_1 (1,2-DCP)$+(1-x_1)$ 2-propanol; (–··), x_1 (2-propanol)$+(1-x_1)$ 2-butanol.

gen bonding of 2-alkanols against the formation of hydrogen bonds between 2-propanol and 2-butanol molecules during mixing process. The maximum values of $H^E_{m,12}$, $H^E_{m,13}$ and $H^E_{m,1+23}$ occur near x_1=0.55-0.6, and at constant composition of x_1, the excess enthalpies $H^E_{m,1+23}$ of the pseudobinary mixtures increase gradually with an increase of the relative amount of the 2-butanol in the binary mixture composed of {2-propanol (2)+2-butanol (3)}.

Experimental results of $H^E_{m,123}$ for the ternary system were correlated as the sum of binary and ternary contributions:

$$H^E_{m,123}(\mathrm{J/mol})=H^E_{m,bin}+x_1x_2(1-x_1-x_2)\Delta_{123} \tag{4}$$

where $H^E_{m,bin}$, as the binary contribution to the excess molar enthalpy of a ternary system, is expressed by:

$$H^E_{m,bin}(\mathrm{J/mol})=\sum_{i=1}^{2}\sum_{j=2}^{3}H^E_{m,ij}=H^E_{m,12}+H^E_{m,13}+H^E_{m,23} \tag{5}$$

where $H^E_{m,ij}$ (i<j) is the binary excess enthalpies calculated from the correlation (by Eq. (2)) of the constituting binary combination i-j pairs using the ternary mole fractions. Several correlations for the ternary contribution are suggested in the literature. In this work, and the ternary contribution term Δ_{123} to excess molar enthalpy of the ternary system was fitted to the expression suggested by Morris et al. [9]:

$$\frac{\Delta_{123}}{RT}=c_0+c_1x_1+c_2x_2+c_3x_1^2+c_4x_1x_2+c_5x_2^2$$
$$+c_6x_1^3+c_7x_1^2x_2+c_8x_1x_2^2+c_9x_2^3\cdots \tag{6}$$

The parameters c_i of Eq. (6) computed by the unweighted least-squares method using a non-linear regression procedure similar to that for the binary parameters are listed in Table 5. The optimal number of the parameters, c_i, was also determined with an optimization algorithm similar to that of the binary systems. The lines of constant ternary excess molar enthalpy, $H^E_{m,123}$, calculated using Eqs. (4)-(6), are presented in Fig. 5. Most of the ternary $H^E_{m,123}$ values show endothermic effects, except with the solutions at a very small molar fraction of 1,2-DCP, where there is an influence of the exothermic effect of 2-propanol (2)+2-butanol (3) system. The maximum value is 1966.1 J/mol. Excess molar enthalpies $H^E_{m,123}$ for this ternary system were also predicted using the Radojkovič equation [22] as shown by Eq. (7), which is used with only binary contributions evaluated by Redlich-Kister equation.

$$H^E_{m,123}(\mathrm{J/mol})=H^E_{m,12}{}^*+H^E_{m,13}{}^*+H^E_{m,23}{}^* \tag{7}$$

where $H^E_{m,12}{}^*$, $H^E_{m,13}{}^*$, and $H^E_{m,23}{}^*$ represent the excess molar enthalpies with x_1, x_2, and x_3 (mole fractions of the ternary mixture) calculated from Eq. (2) using the parameters in Table 3. The standard deviations between experimental and predicted $H^E_{m,123}$ values are given in Table 6. For this ternary system, the $H^E_{m,123}$ values predicted by an equation having both binary and ternary contribution terms show better results than that of having binary contribution terms only.

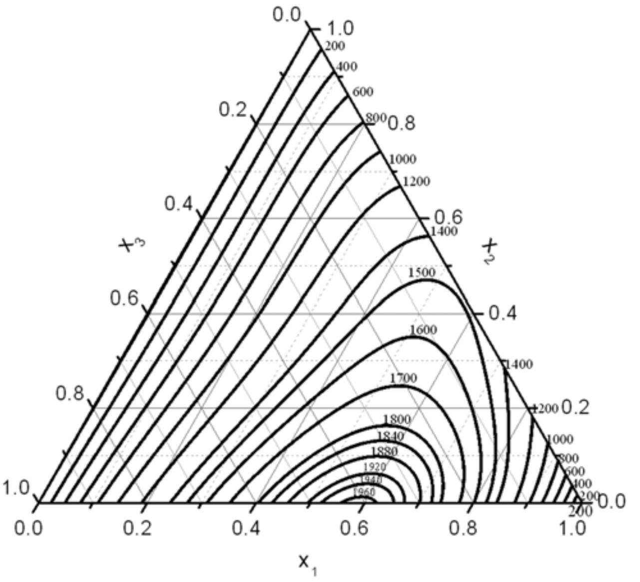

Fig. 5. Lines of constant excess molar enthalpies $H^E_{m,123}$ (J/mol) for ternary mixture {x_1 (1,2-DCP)+x_2 (2-propanol)+x_3 (2-butanol)} at T=298.15 K calculated from correlation of the experimental results by Eq. (4) using parameters listed in Tables 3 and 5.

Table 6. Standard deviation (by Eq. (3)) and RMSD[a] (root mean square deviation) in the prediction of with the predictive models for the ternary system

Predictive model	σ (J/mol)	RMSD (J/mol)
This work using Morris model	25.3	15.3
Radojkovič equation	82.1	63.2

$$^a\mathrm{RMSD}=\sqrt{\frac{\sum(H^E_{123(exp)i}-H^E_{123(calc)i})^2}{N}}$$

CONCLUSIONS

Experimental excess molar enthalpies for the binary and ternary mixtures of 1,2-DCP, 2-propanol, and 2-butanol at T=298.15 K and atmospheric pressure were measured using an isothermal flow-calorimeter. The $H^E_{m,ij}$ values for the binary mixtures {1,2-DCP+2-alkanols} show an endothermic effect (positive values), which exhibits a regular increase with an increase of alkyl-chain length of 2-alkanols, while the binary mixture {2-propanol+2-butanol} is formed slightly exothermally (negative values) over the whole range of composition. The ternary system shows endothermic behavior over the

Table 5. Fitting parameters c_i for ternary contribution in Eq. (6) and standard deviation

Ternary system	c_0	c_1	c_2	σ (J/mol)
	c_3	c_4	c_5	
x_1 (1,2-DCP)+x_2 (2-propanol)	−0.2196	4.7854	−9.5546	17.4
+(1−x_1−x_2) 2-butanol	−11.8927	0.9723	15.7196	

whole ternary composition range with a maximum value $H^E_{m,123}$= 1,966.1 J/mol. The Redlich-Kister equation was used to correlate the binary $H^E_{m,ij}$ data, while the Morris equation was employed to correlate the ternary $H^E_{m,123}$ data. In the case of three pseudobinary mixtures, $H^E_{m,1+23}$ shows all positive values and the magnitude in $H^E_{m,1+23}$ increases gradually with an increase of the relative amount of the 2-butanol in the binary mixture composed of {2-propanol (2)+2-butanol (3)}. Ternary predictions using the Morris equation show better agreement with experimental data for this ternary system; the Morris model using ternary contribution term is obviously superior to the Radojkovič model (not containing ternary contribution term).

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NOMENCLATURE

List of Symbols

A_j, c_i : adjustable parameters for Redlich-Kister and Morris equation, respectively
$H^E_{m,ij}$, $H^E_{m,1+23}$, and $H^E_{m,123}$: excess molar enthalpy of binary, pseudobinary, and ternary systems, respectively [J/mol]
n : number of adjustable parameters
N : number of experimental data points
n_D^{25} : refractive index at T=298.15 K
P : pressure [kPa]
R : universal gas constant [J/mol K]
T : temperature [K]
x_i : liquid mole fraction of component i

Greek Letters

Δ_{123} : ternary contribution term
ρ : density [g/cm^3]
σ : standard deviation [J/mol]

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