

Densities and viscosities of the binary mixtures of phenylmethanol with 2-butanone

メタデータ	言語: English 出版者: 公開日: 2017-10-03 キーワード (Ja): キーワード (En): 作成者: Habibullah, M., Rahman, Ismail M. M., Uddin, M. Ashraf, Iwakabe, Koichi, Azam, Anisul, Hasegawa, Hiroshi メールアドレス: 所属:
URL	http://hdl.handle.net/2297/29311

1 Densities and Viscosities of the Binary Mixtures of
2 Phenylmethanol with 2–Butanone
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1 **Abstract**

2 Densities and viscosities of the binary systems of phenylmethanol with 2-butanone were measured for
3 the entire composition range at $T = (303.15, 308.15, 313.15, 318.15 \text{ and } 323.15)$ K and at the
4 atmospheric pressure. The excess molar volumes were derived from the experimental data, and were
5 fitted with the Redlich–Kister equation to obtain their coefficients and standard deviations. The
6 Grunberg–Nissan equation was used to correlate the viscosity data. Furthermore, kinematic viscosities
7 were compared with those predicted by UNIFAC–VISCO model. The cause of relatively large
8 deviations between the experimental and predicted kinematic viscosities was explored by comparing
9 combinatorial and residual term of UNIFAC–VISCO model.

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1 **Introduction**

2 The fluid property data are essential to explore their usability in the analytical applications that work
3 with mixed solvents, process engineering design applications and other related areas, and have drawn
4 considerable interest in recent years. We are interested in the accumulation of the physical property data
5 of organic liquid mixtures,¹⁻⁵ and as a continuation of our effort, we are reporting here the density and
6 viscosity data of the binary mixtures of phenylmethanol with 2-butanone at $T = (303.15, 308.15, 313.15,$
7 318.15 and $K. 3.15)$ K.

8 Phenylmethanol is a polar solvent with strong self-associating nature via hydrogen bonding, while 2-
9 butanone is an aprotic and protophilic solvent, and both the liquids are widely used as a solvent in the
10 laboratory and industrial processes. In this study, density and viscosity of the binary liquid mixtures of
11 different compositions covering the entire range were measured. The experimental density data were
12 used to derive the excess molar volume, V_m^E , and Redlich-Kister type polynomial equation⁶ was used to
13 estimate the binary coefficients and the standard deviations. The Grunberg-Nissan interaction parameter
14 which indicates the strength of interactions of the components was calculated using the correlation
15 equation.⁷ Kinematic viscosities for the binary system predicted by UNIFAC-VISCO model^{8, 9} were
16 compared with the experimental values. The experimental data and the derived quantities were used to
17 understand the likely interactions of the $>C=O$ group of 2-butanone either with the $-OH$ group of
18 phenylmethanol or with the delocalized π -electrons the benzene ring in phenylmethanol.

19 Our survey of the literature shows that there have not been any density or viscosity data reported for
20 the binary system of phenylmethanol with 2-butanone.

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22 **Experimental**

23 Phenylmethanol (Aldrich, 0.99 mass fraction purity) and 2-butanone (Aldrich, >0.99 mass fraction
24 purity) were used without additional treatment. Density and viscosity data from literatures have been
25 used to ascertain the solvent purity (Table 1).

1 An analytical balance (Model: B 204–S, Mettler Toledo, Switzerland) with uncertainty of ± 0.0001 g
2 was used to prepare the binary mixtures. Mixtures were prepared by mass just before use, and were
3 completely miscible over the entire composition range. The uncertainty in the mole fraction was less
4 than $\pm 1 \cdot 10^{-4}$. A 25 mL specific gravity bottle and A–type Ostwald viscometer, previously calibrated
5 with redistilled water, were used for the measurement of density and viscosity correspondingly. The
6 mean uncertainties in densities and viscosities, respectively, were estimated to be $0.0004 \text{ g} \cdot \text{cm}^{-3}$ and \pm
7 0.5%. A thermostatic water bath equipped with the Thermo Haake DC10 controller (Thermo Fisher
8 Scientific, MA, USA) was used to maintain the temperatures with an average uncertainty of ± 0.05 K.

9 All the measurements were conducted in triplicate and averaged for calculations. LAB Fit¹⁰ and LSM
10 ¹¹ curve–fitting programs were used for least–square regression analyses.

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12 **Results and Discussion**

13 Experimental densities, ρ_{exp} and excess molar volume, V_{m}^{E} for different binary compositions of
14 phenylmethanol with 2–butanone at $T = (303.15, 308.15, 313.15, 318.15 \text{ and } 323.15)$ K is listed in
15 Table 2. Excess molar volumes were calculated using the following relation:

$$16 \quad V_{\text{m}}^{\text{E}} = \left[(x_1 M_1 + x_2 M_2) / \rho_{\text{exp}} - \left\{ (x_1 M_1) / \rho_1 + (x_2 M_2) / \rho_2 \right\} \right] \quad (1)$$

17 where ρ_{exp} is for density of the binary mixtures. The mole fraction, molar mass and density of
18 phenylmethanol are represented with x_1, M_1 and ρ_1 , and the corresponding quantities of 2–butanone are
19 denoted with x_2, M_2 and ρ_2 , respectively. Excess molar volume, V_{m}^{E} of the (phenylmethanol + 2–
20 butanone) system as a function of the binary compositions at $T = (303.15, 308.15, 313.15, 318.15 \text{ and}$
21 $323.15)$ K is shown in Figure 1. The V_{m}^{E} values are negative throughout the composition range,
22 decreases with an increase in phenylmethanol concentration up to the mole fraction, $x_1 \approx 0.5$, and then
23 increases further with the change in x_1 . Such behavior may be accounted to the change in orientation of
24 the molecules within the mixtures due to the interaction between the components with the addition of
25 H–bonding containing liquid into the system, and partial interstitial accommodation of ketone molecules

1 into the network of alcohol at the phenylmethanol-rich conditions. It is assumed that the latter effect not
 2 only compensates the former effect but also predominates largely, resulting in a net negative V_m^E . There
 3 are two probable pathways, which may result from the change in orientation of the molecules within the
 4 mixtures – (a) interaction between the –OH group of phenylmethanol and the >C=O group of 2-
 5 butanone through H-bonding (*i.e.* –O–H.....O=C<) and (b) interaction between the delocalized π -
 6 electrons of the benzene ring in phenylmethanol with the >C=O group of 2-butanone.¹² Decreasing
 7 trend in the variations of V_m^E values is observed with the rise of temperatures, *i.e.* $\partial V_m^E/\partial T < 0$. Greater
 8 population of intermolecular complex within the system, which is attributable to the increasing
 9 proportion of smaller multimers as well as the monomers of phenylmethanol and 2-butanone with the
 10 increase in temperature, is thus supposed to explain such behavior.

11 The composition dependence of V_m^E can be represented by a Redlich–Kister type equation:⁶

$$12 \quad Y = x_1 x_2 \sum_{i=0}^n A_i (1 - 2x_1)^i \quad (2)$$

13 where Y refers to V_m^E , and the mole fractions of phenylmethanol and 2-butanone are represented with x_1
 14 and x_2 , respectively. The coefficients A_i in eq 2 were obtained by fitting the equation with the
 15 experimental values (Table 4). The standard deviation values, as listed in Table 3, were calculated from
 16 the following equation:

$$17 \quad \sigma(Y) = \left[\sum (Y_{\text{expt}} - Y_{\text{calc}})^2 / (n - p) \right]^{1/2} \quad (3)$$

18 where n is the number of experimental points, p is the number of coefficients of eq 2, and Y_{expt} and Y_{calc}
 19 are the experimental and calculated values of the properties.

20 Table 4 lists the experimental viscosities, η_{exp} for different binary compositions at $T = (303.15, 308.15,$
 21 $313.15, 318.15$ and $323.15)$ K. Figure 2 represents the variation of η_{exp} against the mole fraction of
 22 phenylmethanol (x_1) at different temperatures. The viscosity of a mixture strongly depends on the
 23 structure of liquids and bond enthalpy, and consequently, on the molecular interactions between the
 24 components of the mixture.¹³ A gradual increase in the viscosity of the mixtures can be observed with

1 the increasing concentration of phenylmethanol in the binary mixtures with 2–butanone which indicate
 2 the formation of more and more flow-resistant species within the system as the proportion of x_1
 3 increases. The magnitude of η_{exp} decreases as the temperature is higher and such temperature effect on
 4 viscosities is a common phenomenon.¹⁴

5 Viscosity data was analyzed based on the Grunberg–Nissan treatment⁷ whose parameter gives
 6 qualitative information about molecular interactions:

$$7 \quad \eta_{\text{mix}} = \exp(x_1 \ln \eta_1 + x_2 \ln \eta_2 + x_1 x_2 d) \quad (4)$$

8 where d is an interaction parameter that is a function of the nature of the components and temperature,
 9 and has been regarded as a measure of the strength of molecular interactions between the mixture
 10 components. The Grunberg–Nissan interaction parameter (d) values are found to be negative and quite
 11 large in magnitude for the whole range of composition, and decrease with the increase of temperature
 12 (Table 5). According to Fort and Moore,¹⁵ such pattern in d values indicate the tendency of the systems
 13 to move towards more ideal conditions, which are due to the absence of specific interaction and
 14 presence of dominant dispersive force between the components.

15 In this study, kinematic viscosities were calculated with the experimental density and viscosity data,
 16 and compared with those predicted by UNIFAC–VISCO model.^{8,9} In UNIFAC–VISCO model, the
 17 relationship between the kinematic viscosity and the excess Gibbs energy of activation, Δ^*G^E is
 18 expressed in the following form:

$$19 \quad \ln(\nu M) = \sum_i^{NC} x_i \ln(\nu_i M_i) + \frac{\Delta^*G^E}{RT} \quad (5)$$

$$20 \quad \Delta^*G^E = \Delta^*G^{\text{EC}} + \Delta^*G^{\text{ER}} \quad (6)$$

21 where M is molecular weight, Δ^*G^E , Δ^*G^{EC} and Δ^*G^{ER} are excess Gibbs energy of activation and its
 22 combinatorial and the residual parts, respectively. In UNIFAC-VISCO model, the combinatorial part
 23 expresses the contribution of shape differences among molecules to the Δ^*G^E , while the residual part
 24 accounts for the enthalpy effect caused by mixing. In Figure 3, kinematic viscosities predicted by

1 UNIFAC-VISCO model are compared with the experimental ones. For the prediction, the interaction
 2 parameters reported by Gaston-Bonhomme et al.⁹ are used. Experimental kinematic viscosities, v_{exp} ,
 3 experimental viscosities, η_{exp} , and experimental densities, ρ_{exp} , in Table 2 and 4 have the following
 4 relationship:

$$5 \quad v_{\text{exp}} = \frac{\eta_{\text{exp}}}{\rho_{\text{exp}}} \quad (7)$$

6 As can be seen from the figure, the kinematic viscosities obtained by UNIFAC-VISCO model are
 7 smaller than the experimental ones at all temperatures. The relative errors, $E_{v,i}$, and the absolute average
 8 differences, AAD, was expressed by the following equations, and shown in Table 6:

$$9 \quad E_{v,i} = \frac{v_{\text{exp},i} - v_{\text{cal},i}}{v_{\text{exp},i}} \times 100 \quad (8)$$

$$10 \quad \text{AAD} = \frac{1}{n} \sum_i^{N_p} |E_{v,i}| \quad (9)$$

11 where i denotes the i -th experimental data and n is the number of the experimental data at each
 12 temperature. In order to explore the cause of the deviations, Δ^*G^E , Δ^*G^{EC} , Δ^*G^{ER} , and Δ^*G^E from the
 13 experimental data were also compared with each other. The experimental Δ^*G^E was obtained by the
 14 following equation:

$$15 \quad \left. \frac{\Delta^*G^E}{RT} \right|_{\text{exp}} = \ln(v_{\text{exp}}M) - \sum_i^{NC} x_i \ln(v_i M_i) \quad (10)$$

16 where NC is the number of components. Since the results of comparisons were similar at all
 17 temperatures, that at 303.15 K is shown in Figure 4 as an example. As can be seen from the figure, the
 18 absolute values for $\Delta^*G^E_{\text{exp}}$ are much smaller than the predicted ones. Since absolute values for the
 19 combinatorial part are smaller than those for the residual part, the residual part seems to be responsible
 20 for the large deviation. The greater absolute values of the residual term mean the individual
 21 contributions of constituent groups in the system are overestimated by UNIFAC-VISCO model.

22

1 **Conclusions**

2 Densities and viscosities for the binary mixtures of phenylmethanol with 2-butanone have been
3 determined experimentally as a function of temperature and at the atmospheric pressure. Excess molar
4 volumes have been derived from the experimental density data, and the patterns are negative throughout
5 the composition range. Analysis of viscosity data based on the Grunberg–Nissan treatment show that no
6 specific interaction exists among the component molecules. Furthermore, experimental kinematic
7 viscosities were obtained by densities and viscosities, and compared with those predicted by UNIFAC–
8 VISCO model. The deviations between experimental and predicted kinematic viscosities are large, and
9 larger the temperature higher. By the comparisons among excess Gibbs energies of activation, the
10 residual term in UNIFAC–VISCO model seems to be responsible for those large deviations.

11

12 **Acknowledgment**

13 The authors are grateful to the Kanazawa University authorities for providing the necessary
14 opportunities to accomplish the research work. Additionally, I.M.M.R. acknowledges the support from
15 the Japanese Government (Monbukagakusho: MEXT) Scholarship program that facilitated this research.

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1 **Table 1. Comparison of Experimental Densities, ρ_{exp} and Viscosities, η_{exp} of Pure Solvents with**
 2 **Literature Values at $T = (303.15, 308.15, 313.15, 318.15 \text{ and } 323.15) \text{ K}$**

Component	T/K	$\rho/\text{g}\cdot\text{cm}^{-3}$			$\eta/\text{mPa}\cdot\text{s}$		
		Exp.	Lit.	Ref.	Exp.	Lit.	Ref.
Phenylmethanol	303.15	1.0376	1.0376	¹⁶	4.689	4.670	¹⁷
	308.15	1.0338	1.0337	¹⁷	4.058	4.004	¹⁷
						4.093	¹⁸
	313.15	1.0301	1.0294	¹⁷	3.531	3.530	¹⁹
	318.15	1.0263	1.02572	²⁰	3.103	3.120	²⁰
	323.15	1.0225	1.0221	¹⁶	2.747		
2-Butanone	303.15	0.7940	0.7944	²¹	0.362	0.3653	²²
						0.366	²³
	308.15	0.7888	0.7888	²⁴	0.345	0.3441	²⁴
						0.3440	²²
	313.15	0.7835	0.7831	²⁵	0.330		
	318.15	0.7783	0.7785	²⁶	0.316	0.311	²⁶
323.15	0.7730	0.7733	¹	0.303			

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1 **Table 2. Composition, Experimental Densities, ρ_{exp} and Excess Molar Volumes, V_{m}^{E} for the**
2 **Binary Mixtures of Phenylmethanol (1) with 2-Butanone (2) at $T = (303.15, 308.15, 313.15, 318.15$**
3 **and $323.15)$ K**

	$T/\text{K} = 303.15$		$T/\text{K} = 308.15$		$T/\text{K} = 313.15$		$T/\text{K} = 318.15$		$T/\text{K} = 323.15$	
x_1	ρ_{exp} /g·cm ⁻³	V_{m}^{E} /cm ³ ·mol ⁻¹	ρ_{exp} /g·cm ⁻³	V_{m}^{E} /cm ³ ·mol ⁻¹	ρ_{exp} /g·cm ⁻³	V_{m}^{E} /cm ³ ·mol ⁻¹	ρ_{exp} /g·cm ⁻³	V_{m}^{E} /cm ³ ·mol ⁻¹	ρ_{exp} /g·cm ⁻³	V_{m}^{E} /cm ³ ·mol ⁻¹
0.0000	0.7940	0.0000	0.7888	0.0000	0.7835	0.0000	0.7783	0.0000	0.7730	0.0000
0.1003	0.8254	-0.4210	0.8204	-0.4389	0.8154	-0.4670	0.8104	-0.4862	0.8053	-0.5053
0.2000	0.8547	-0.6994	0.8499	-0.7308	0.8451	-0.7706	0.8403	-0.8042	0.8355	-0.8484
0.3010	0.8825	-0.8528	0.8778	-0.8833	0.8730	-0.9090	0.8683	-0.9415	0.8636	-0.9835
0.3991	0.9075	-0.8623	0.9030	-0.9000	0.8984	-0.9312	0.8939	-0.9712	0.8893	-1.0087
0.5001	0.9326	-0.8790	0.9282	-0.9118	0.9238	-0.9463	0.9194	-0.9812	0.9150	-1.0232
0.6000	0.9563	-0.8491	0.9520	-0.8758	0.9478	-0.9123	0.9436	-0.9513	0.9393	-0.9856
0.7008	0.9782	-0.6816	0.9741	-0.7103	0.9699	-0.7258	0.9658	-0.7561	0.9617	-0.7908
0.8001	0.9985	-0.4529	0.9946	-0.4827	0.9905	-0.4868	0.9856	-0.4141	0.9827	-0.5522
0.8997	1.0181	-0.2091	1.0143	-0.2292	1.0104	-0.2315	1.0065	-0.2420	1.0027	-0.2645
1.0000	1.0376	0.0000	1.0338	0.0000	1.0301	0.0000	1.0263	0.0000	1.0225	0.0000

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1 **Table 3. Coefficients, A_i , of Redlich–Kister Equation (Equation 2), Expressing Excess Molar**
 2 **Volumes, V_m^E and Standard Deviation, σ for the Binary Mixtures of Phenylmethanol (1) with 2–**
 3 **Butanone (2) at $T = (303.15, 308.15, 313.15, 318.15$ and $323.15)$ K**

T/K	A_0	A_1	A_2	A_3	σ
303.15	–3.5764	–0.6174	–0.0394	–1.5488	0.0204
308.15	–3.7035	–0.6727	–0.1846	–1.4255	0.0186
313.15	–3.8312	–0.6856	–0.2004	–1.7601	0.0199
318.15	–3.9907	–0.8351	0.1331	–2.0097	0.0385
323.15	–4.1379	–0.7466	–0.4488	–1.7385	0.0222

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1 **Table 4. Composition and Experimental Viscosities, η_{exp} for the Binary Mixtures of**
 2 **Phenylmethanol (1) with 2-Butanone (2) at $T = (303.15, 308.15, 313.15, 318.15$ and $323.15)$ K**

x_1	$\eta_{\text{exp}} / \text{mPa}\cdot\text{s}$				
	$T/\text{K} = 303.15$	$T/\text{K} = 308.15$	$T/\text{K} = 313.15$	$T/\text{K} = 318.15$	$T/\text{K} = 323.15$
0.0000	0.362	0.345	0.330	0.316	0.303
0.1003	0.446	0.424	0.403	0.385	0.368
0.2000	0.554	0.524	0.497	0.472	0.451
0.3010	0.697	0.655	0.616	0.582	0.551
0.3991	0.876	0.818	0.765	0.718	0.676
0.5001	1.131	1.046	0.970	0.904	0.845
0.6000	1.476	1.351	1.242	1.146	1.063
0.7008	1.947	1.761	1.599	1.461	1.341
0.8001	2.586	2.307	2.063	1.866	1.694
0.8997	3.452	3.033	2.682	2.391	2.144
1.0000	4.689	4.058	3.531	3.103	2.747

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1 **Table 5. Grunberg–Nissan Interaction Parameters (d) for the Binary Mixtures of Phenylmethanol**
 2 **(1) with 2–Butanone (2) at $T = (303.15, 308.15, 313.15, 318.15$ and $323.15)$ K**

x_1	$T/K = 303.15$	$T/K = 308.15$	$T/K = 313.15$	$T/K = 318.15$	$T/K = 323.15$
0.1003	-0.540	-0.474	-0.413	-0.358	-0.317
0.2000	-0.535	-0.470	-0.406	-0.352	-0.279
0.3010	-0.550	-0.483	-0.422	-0.368	-0.314
0.3991	-0.575	-0.507	-0.439	-0.380	-0.324
0.5001	-0.564	-0.497	-0.429	-0.370	-0.312
0.6000	-0.545	-0.476	-0.405	-0.344	-0.285
0.7008	-0.535	-0.466	-0.396	-0.334	-0.277
0.8001	-0.518	-0.453	-0.399	-0.325	-0.269
0.8997	-0.547	-0.487	-0.413	-0.350	-0.298

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1 **Table 6. Comparison of the Experimental and Calculated Values of the Kinematic Viscosity**

T/K	AAD/%	$ E_v _{\max}/\%$	$ \Delta v/v _{\max} \times 100$
303.15	12.27	19.3	15.9
308.15	13.01	20.5	14.0
313.15	13.73	21.7	12.2
318.15	14.37	22.7	10.6
323.15	14.95	23.7	9.0

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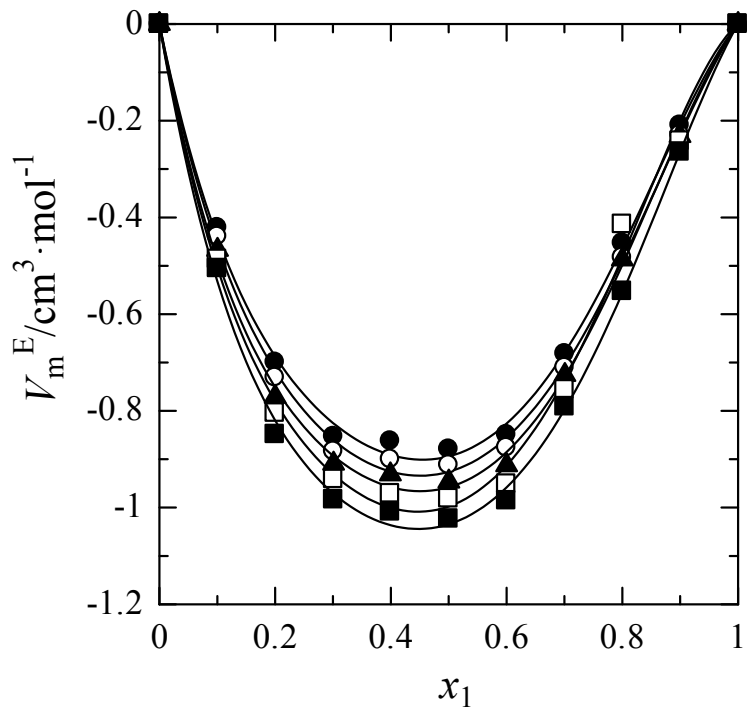
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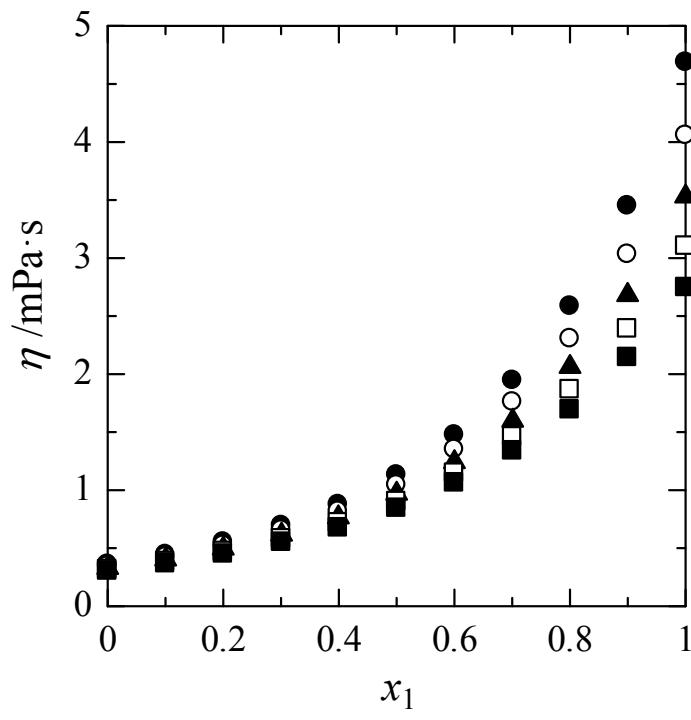
2 **Figure 1.** Excess molar volumes for the system phenylmethanol (1) + 2-butanone (2): ●, 303.15 K; ○,

3 308.15 K; ▲, 313.15 K; □, 318.15 K; ■, 323.15 K.

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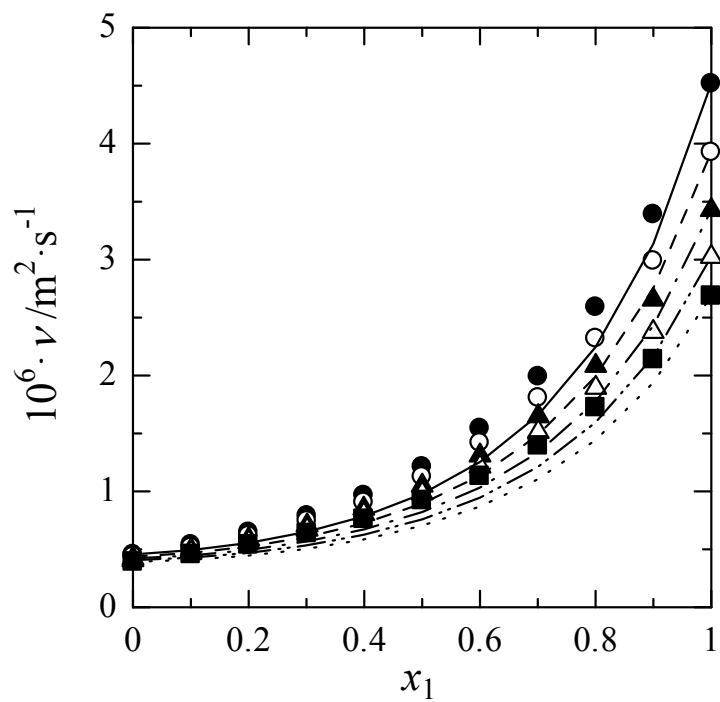
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2 **Figure 2.** Experimental viscosities for the system phenylmethanol (1) + 2-butanone (2): ●, 303.15 K;

3 ○, 308.15 K; ▲, 313.15 K; □, 318.15 K; ■, 323.15 K.

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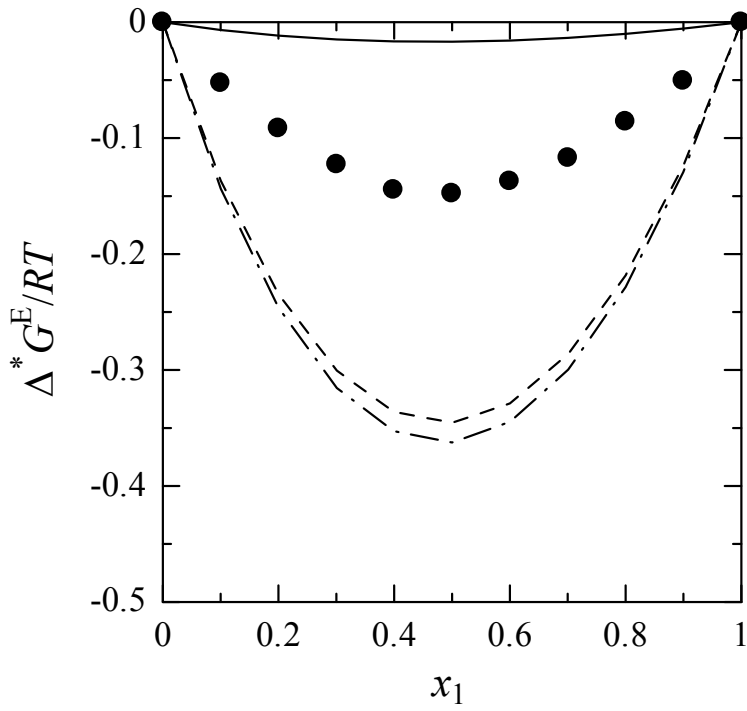
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2 **Figure 3.** Kinematic viscosities for the system phenylmethanol (1) + 2-butanone (2): ●, ν_{exp} at 303.15

3 K; ○, ν_{exp} at 308.15 K; ▲, ν_{exp} at 313.15 K; □, ν_{exp} at 318.15 K; ■, ν_{exp} at 323.15 K ; —, ν_{cal} at 303.15

4 K; - - -, ν_{cal} at 308.15 K; - · - · -, ν_{cal} at 313.15 K; - · · - · -, ν_{cal} at 318.15 K; ·····, ν_{cal} at 323.15 K.

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2 **Figure 4.** Excess Gibbs energy of activation for the system phenylmethanol (1) + 2-butanone (2) at $T =$

3 303.15 K: ●, $\Delta^*G^E_{\text{exp}}/RT$; —, $\Delta^*G^{\text{EC}}_{\text{cal}}/RT$; - - , $\Delta^*G^{\text{ER}}_{\text{cal}}/RT$; - · -, $\Delta^*G^E_{\text{cal}}/RT$.

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