Volumetric Properties, Viscosities, and Refractive Indices for Aqueous 1-Amino-2-Propanol (Monoisopropanolamine (MIPA)) Solutions from (298.15 to 343.15) K

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Densities and viscosities at six temperatures in the range (298.15 to 343.15) K and refractive indices at nine temperatures in the range (293.15 to 333.15) K are reported for aqueous solutions of 1-amino-2-propanol (monoisopropanolamine (MIPA) or 1-AP). Excess molar volumes, viscosity deviations, and refractive index deviations were calculated from the measurement results and correlated as a function of composition using the Redlich−Kister relation and polynomial equations. Partial molar volumes at infinite dilution were determined from the apparent molar volumes. Negative values for excess molar volumes and molar refraction changes are observed over the whole composition range, whereas viscosity data exhibit both negative and positive deviations. Cross-associated hydrogen bonds forming between 1-AP and water contribute to the deviations in the properties with respect to mole fractions and temperatures.

Introduction

1-Amino-2-propanol ($CH_3(CH)OH(CH_2)NH_2$, 1-AP or MIPA) is a primary hindered amine used as an absorbent of acid gases in the refinery of natural gas and purification of ammonia. It is soluble in water and has a low alkalinity. It is used as a cross-linking catalyst in the production of polyurethanes, an emulsifying agent, and a component of insecticides, surfactants, rubber chemicals, corrosion inhibitors, and pigment dispersants. 1-AP, which is a primary alkanolamine having ($-NH_2$ and $-OH$) functional groups, showed a similar behavior to that of monoethanolamine (MEA) in absorbing CO_2.[1,2]

The removal of acid gases such as carbon dioxide and hydrogen sulfide from gas streams in natural gas and petroleum industries are being carried out using aqueous alkanolamines. Alkanolamines are of increasing importance in treating acidic gas streams in various chemical production industries. The knowledge of physical properties such as densities, viscosities, and refractive indices is required for engineering design and subsequent operations as summarized by Astarita et al.[1] The estimated accuracy of physical properties of mixtures affects the reliability of process design calculations for designing the equipment. In addition, volumetric data combined with molecular theories or models are used to extend our understanding of molecular interactions in the absorption system. Camacho et al.[3] studied the absorption of CO_2 at high partial pressures in 1-AP aqueous solution and suggested that it can be used as an absorbent for capturing carbon dioxide from postcombustion exhaust gases. The net cyclic capacity and reaction rate of 1-AP with CO_2 is similar to that of MEA. The solubility and diffusivity of gases in aqueous solutions of 1-AP were reported by Sada et al. using a laminar jet.[4] The reaction mechanism and kinetics of these amines were studied and compared with other primary amines by Bavbek and Alper[5] and Penny and Ritter[6] at 303 K. Hikita et al.[7] studied the kinetics of 1-AP in the concentration ranges from (16.8 to 46.4) $mol \cdot m^{-3}$ from (278.7 to 313.6) K and concluded that it has an absorption rate similar to MEA. The reaction kinetics of 1-AP was compared with 3-amino-1-propanol and MEA by Henni et al.[8] Densities, viscosities, and diffusivities of aqueous 1-AP at 298 K were published by Hikita et al.[9] Volumetric properties of the (1-AP + water) mixture at atmospheric pressure from (283.15 to 353.15) K were reported by Mokraoui et al.[10] In this work we provided data for viscosities and refractive indices for the binary systems of 1-AP (1) + water (2). No literature data of viscosities and refractive indices were available for 1-AP (1) + water (2) for the temperature range from (298.15 to 343.15) K. We also provide experimental data for densities for the (1-AP + water) mixture at atmospheric pressure from (283.15 to 353.15) K, and derived molar volumes were compared with those of Mokraoui et al.[10] From apparent molar volumes, partial molar volumes at infinite dilution were determined. From the experimental viscosity and refractive index data, viscosity deviations and refractive index deviations were calculated. Redlich−Kister equation and polynomial equations were used to fit the calculated binary data to express all of the physical properties.

Experimental Section

1-AP (weight fraction = 0.99) was purchased from Sigma Aldrich and was used without further purification. An analytical balance Ohaus (model Ap 205 D, Florham Park, NJ) was used to prepare gravimetrically the binary mixtures of 1-AP and deionized water with a precision of ± 0.1 mg. The overall possible uncertainty in the mass fractions is around ± 0.0001. Densities of the binary mixtures were measured with an Anton Paar DMA-4500 density meter. Air and water were used to calibrate the apparatus at ambient temperature. The densities were measured for deionized water which was distilled using by a distiller (model A1007, Barnstead Thermo Scientific, USA) in the temperature range (279.15 to 353.15) K and were compared with the values measured by Bettin and Spieweck[11] and with the values in the annual book of ASTM standards.[12] The densities of air were compared with the values from the annual book of ASTM standards.[12] The calibration was accept-

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10.1021/je100300s

Table 1. Density, ρ/g·cm^{-3}, for 1-AP (1) + Water (2) Mixtures from (298.15 to 343.15) K

	T/K					
x_1	298.15	303.15	313.15	323.15	333.15	343.15
0	0.99704	0.99564	0.99221	0.98803	0.98319	0.97775
0.0500	0.99990	0.99707	0.99268	0.98766	0.98203	0.97562
0.0700	1.00035	0.99810	0.99309	0.98741	0.98149	0.97499
0.0986	1.00243	0.99983	0.99425	0.98820	0.98157	0.97344
0.1993	1.00457	1.00103	0.99372	0.98618	0.97850	0.97055
0.3003	0.99991	0.99608	0.98829	0.98032	0.97215	0.96377
0.3955	0.99294	0.98908	0.98119	0.97313	0.96488	0.95645
0.4929	0.98582	0.98192	0.97392	0.96584	0.95768	0.94925
0.5995	0.97802	0.97420	0.96630	0.95838	0.95015	0.94171
0.7002	0.97166	0.96774	0.95983	0.95177	0.94353	0.93509
0.8006	0.96596	0.96201	0.95401	0.94587	0.93762	0.92919
0.8992	0.96108	0.95712	0.94912	0.94096	0.93266	0.92420
1.0000	0.95651	0.95252	0.94442	0.93619	0.92784	0.91937

Table 2. Viscosity, η/mPa·s, for 1-AP (1) + Water (2) Mixtures from (298.15 to 343.15) K

	T/K					
x_1	298.15	303.15	313.15	323.15	333.15	343.15
0	0.882	0.804	0.658	0.551	0.470	0.407
0.0500	2.110	1.856	1.431	1.136	0.929	0.775
0.0700	2.696	2.282	1.785	1.393	1.118	0.922
0.0986	3.902	3.248	2.359	1.561	1.222	0.993
0.1993	9.700	7.671	5.102	3.582	2.627	2.088
0.3003	15.544	12.040	7.551	5.590	3.944	2.904
0.3955	22.187	16.820	9.950	6.649	4.988	3.619
0.4929	26.762	19.499	11.794	7.640	5.701	4.075
0.5995	29.010	21.376	12.849	7.994	6.163	4.371
0.7002	29.986	22.781	13.135	8.473	5.753	4.565
0.8006	30.403	22.970	13.564	8.748	6.023	4.467
0.8992	28.546	22.191	12.829	8.041	5.483	3.927
1.0000	26.685	20.314	12.514	7.543	5.220	3.770

able if the measurements were within ± $5\cdot10^{-5}$ g·cm^{-3} of the published values. The uncertainty of our density data was estimated to be ± $5\cdot10^{-5}$ g·cm^{-3}. The reproducibility of density measurements was ± $2\cdot10^{-5}$ g·cm^{-3}. U-tube glass Cannon-Ubbelohde viscometers (Cole-Parmer) were used for the measurement of viscosities. To measure the viscosities of aqueous 1-AP at different temperatures, viscometers were placed in a well-stirred constant temperature bath (model CT 500, Cannon Instrument Company, USA). The uncertainty of the water bath temperature was 0.01 K as measured by a Cole-Parmer resistance thermometer (model H-01158-65, Anjou, Quebec, Canada). Viscosities were determined with nine different viscometers to cover, with precision,[13] the range of temperature from (298.15 to 343.15) K. The efflux time was measured with a hand-held certified digital stopwatch capable of measuring time to within 0.01 s. Experiments were repeated a minimum of three times at each temperature for all compositions. The equation for kinematic viscosity, according to Poiseuille's law, is:

$$\nu = k_1 t - k_2/t \qquad (1)$$

where t is the efflux time and k_1 and k_2 are the viscometer constants. The second term in the equation represents the correction due to the kinetic energy and was found to be negligible.[13] The absolute viscosity (η) was obtained by multiplying the measured kinematic viscosity (ν) by the measured density (ρ). Calibration was done as in the previous work using high-purity ethylene glycol and diethylene glycol.[14] Values of the viscosity of water were taken from Stokes and Mills.[15] The uncertainty of the dynamic viscosity is estimated to be less than 1 %. An Atago RX-5000-α refractometer was used to measure the refractive indices of aqueous solutions. The refractive indices of deionized water were measured and compared with the available literature data. The uncertainty in refractive index measurements was found to be ± 0.0001. The refractive indices of 2-(methylamino)ethanol (MAE) and Genosorb 1753 (Selexol) were measured in the temperature range (298.15 to 333.15) K and were compared with the literature.[16,17] The absolute average deviations (AAD) were found to be $2.4\cdot10^{-4}$ and $4.8\cdot10^{-5}$.

Results and Discussion

The measured values of densities and viscosities of the aqueous 1-AP solutions at (298.15 to 343.15) K are listed in Tables 1 and 2 for the whole concentration range. The refractive indices of the aqueous 1-AP solutions at (293.15 to 333.15) K are listed in Table 3 for the entire concentration range. The refractive index was measured to a maximum temperature of 333.15 K because of the limitations of the refractometer.

Densities of pure 1-AP were compared with the experimental values from Mokraoui et al.[10] and the correlations obtained from Daubert et al.[18] and Mokraoui et al.[10] using the equation:

$$\rho^*_{i,\mathrm{corr}} = \frac{A}{B\left(1 + \left(1 - \dfrac{T}{T_\mathrm{c}}\right)^{C}\right)} \cdot \frac{M_i}{1000} \qquad (2)$$

The parameters A (kmol·m^3), B, and C were taken from Mokraoui et al.[10] M_i is the molar mass of pure component i (g·mol^{-1}). T_c is the critical temperature of the pure component i (K). The calculated relative deviations from our experimental values are shown in Figure 1 and were within ± 0.002.

As shown in Figure 2, the density curves increase as 1-AP is added to water, and a maximum occurs at around $x_1 = 0.2$ for all temperatures. The density values measured by Hikita et al.[9] at 298.15 K lie in the density curve obtained in this work which can be observed in Figure 2. The excess molar volume V^E is calculated from the measured density values. The composition dependency of the molar excess volumes at various temperatures is shown in Figure 3. The minimum value for the excess molar volume curves was observed at around ($x_1 = 0.4$) for all temperatures. As the temperature increases, V^E values decreased. Figures 2 and 3 show sharp changes in the density and excess volumes in the water-rich region. Negative excess molar volume values point to a volume contraction and can be explained by the large difference in the molar specific volumes. The volume contraction is due to the ability of the −OH group to form hydrogen bonds with water molecules.[19] Another reason for the decrease in excess molar volumes might be due to the accommodation of the nonaqueous molecules occupying the void spaces in the structured water lattices.[20]

The number of cross-associated H-bonds decreases with increasing temperatures and contributes to a positive V^E. As a consequence, V^E values became more negative with a decrease in temperature.

Figure 4 shows a comparison of the excess volumes of various alkanolamines and indicates that the addition of 1-AP to water brings the increase in the excess volume, lying between 2-((2-aminoethyl)amino)ethanol (AEEA)[20] and diethylglycolamine (DGA),[14] triethanolamine (TEA), MEA, and diethanolamine (DEA).[21]

Table 3. Refractive Index, n_D, for 1-AP (1) + Water (2) Mixtures from (293.15 to 333.15) K

	T/K								
x_1	293.15	298.15	303.15	308.15	313.15	318.15	323.15	328.15	333.15
0	1.33298	1.33249	1.33193	1.33136	1.33067	1.3299	1.32906	1.32818	1.32726
0.0500	1.35692	1.35622	1.35539	1.35453	1.35365	1.35269	1.35169	1.35059	1.35023
0.0700	1.36527	1.36437	1.36345	1.36246	1.36149	1.36047	1.35931	1.35816	1.35711
0.0986	1.3763	1.37524	1.37416	1.37306	1.37191	1.37079	1.36955	1.36821	1.36712
0.1993	1.40333	1.40184	1.40038	1.39868	1.39716	1.39563	1.39469	1.39247	1.39103
0.3003	1.41934	1.41723	1.41554	1.41385	1.41214	1.41051	1.40883	1.4072	1.40563
0.3955	1.42844	1.4268	1.42513	1.42331	1.42155	1.41987	1.41801	1.4164	1.4146
0.4929	1.43452	1.43286	1.431	1.42913	1.4273	1.42548	1.42386	1.4226	1.42038
0.5995	1.43934	1.4377	1.4359	1.43375	1.43187	1.43017	1.42857	1.426973	1.42445
0.7002	1.44298	1.44053	1.43897	1.43685	1.43493	1.43243	1.431463	1.430063	1.42775
0.8006	1.44474	1.44287	1.4411	1.43908	1.43715	1.43532	1.433693	1.431337	1.42949
0.8992	1.44655	1.4447	1.44275	1.44076	1.43889	1.43691	1.4349	1.43292	1.43089
1.0000	1.448	1.44609	1.44409	1.44211	1.44009	1.43817	1.43631	1.43405	1.43208

Excess volume data ($Y(x) = V^E/\mathrm{cm}^3\cdot\mathrm{mol}^{-1}$) were correlated by the Redlich−Kister relation:

$$Y(x) = x_1x_2\sum_{i=0}^{n} a_i(x_1 - x_2)^i \tag{3}$$

The coefficients and the standard deviations are presented in Table 4. The Redlich−Kister relation was used to correlate the unsymmetrical curves of excess volumes (and viscosity deviations). The *F*-test with a 95 % confidence interval was used to determine the optimum number of coefficients. The relative deviations from our experimental values with the Redlich−Kister relation obtained in this work and the relation proposed by Mokraoui et al.[10] were found to be within ± 0.1 $\mathrm{cm}^3\cdot\mathrm{mol}^{-1}$ ($\mathrm{mPa}\cdot\mathrm{s}$ for viscosity deviations), and their trend is shown in Figure 5. Hepler[22] and Neal and Goring[23] explained the usefulness of thermal expansion data to correlate molecular structure of solutes and their effects on water structure. They suggested using the sign of the second derivative of the partial molar volume at infinite dilution of the solute with respect to the temperature ($\mathrm{d}^2V_1^\infty/\mathrm{d}T^2$) to classify solutes as “structure makers” or “structure breakers”. A positive sign is due to a structure-making solute, while a negative sign corresponds to a structure-breaking solute.

Both the partial molar volume of water at infinite dilution (V_2^∞) in 1-AP and the partial molar volume of 1-AP at infinite dilution (V_1^∞) in water were obtained using the method proposed by Maham et al.[24] The apparent molar volume of water ($V_{\phi,2}$) and the apparent molar volume of 1-AP in water ($V_{\phi,1}$) were first calculated as:

$$V_{\phi,2} = V_2^\mathrm{o} + [V^E/(1 - x_1)] \tag{4}$$

$$V_{\phi,1} = V_1^\mathrm{o} + (V^E/x_1) \tag{5}$$

where V_1^0 and V_2^0 are the molar volumes of pure 1-AP and water, respectively. An analytical extrapolation of $V_{\phi,2}$ to $x_1 = 1$ led to V_2^∞, and a similar extrapolation to $x_1 = 0$ led to V_1^∞. Partial molar volumes at infinite dilution are calculated from apparent molar volumes by applying these limits and are listed in Table 5. V_1^∞ values increased linearly with temperature. This shows that the structure of water was not disturbed by the solute 1-AP. This is consistent with the conclusion of Maham et al.[21,24] concerning other alkanolamines (MEA, DEA, and TEA). All of the values of the molar volumes at infinite dilution (V_1^∞) were smaller than the corresponding molar volumes of pure 1-AP (V_1^0). The change in the excess volume is due to the occupancy of 1-AP molecule into the open or empty space in liquid water. This could explain the structure “neutrality”, consistent with the observation that ($\mathrm{d}^2V_1^\infty/\mathrm{d}T^2$) values are equal to zero.

Having fewer values of V^E for x_1 near unity, accuracies of V_2^∞ may be lower. It is still clear that ($\mathrm{d}V_2^\infty/\mathrm{d}T$) is almost zero. All values of V_2^∞ were smaller than the corresponding molar volumes of pure water (V_2^0) at the same temperature. Maham et al.[21] explained that the molar volume of pure water is the sum of the actual molecular volumes plus the “empty” volume that arises from the hydrogen-bonded open structure of water. Values of the apparent molar volumes of 1-AP in water ($V_{\phi,1}$) increased with the increase in temperature and reached a minimum similar to that of Mundhwa et al.[20] and Zhang et al.[25] observed for aqueous AEEA, diethylethanolamine, and dimethyldiethanolamine solutions.

Experimentally measured viscosities of the binary solutions of aqueous 1-AP solutions at (298.15 to 343.15) K are listed in Table 2 and shown in Figure 6. The viscosity values measured by Hikita et al.[9] at 298.15 K lie on the viscosity curve obtained in this work as can be observed in Figure 6. Curves for the system 1-AP + water are S-shaped with a maximum between 0.70 to 0.80 mole fraction. Aqueous AEEA, MDEA,[26] and DGA[14] solutions were also shown to have this S-shaped form. Fort and Moore[27] and Liler and Kosanović[28] explained that an S-shaped viscosity curve and the presence of a maximum are due to the formation of stable complexes. Figure 6 shows a sharp increase in the viscosity of the mixture after the addition

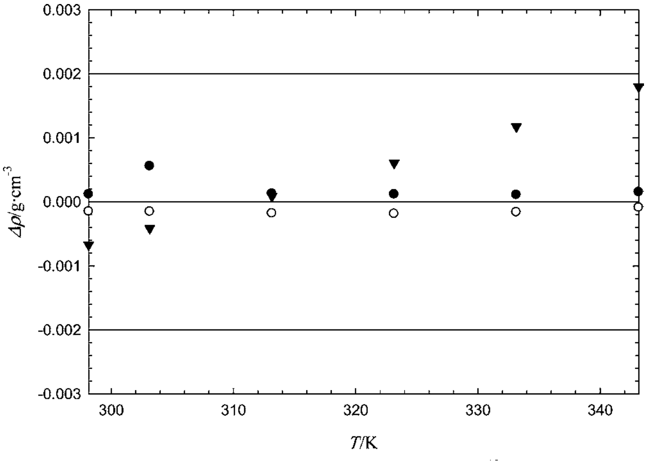

Figure 1. Relative density deviations of pure 1-AP: ●, Mokraoui et al.;[10] ○, correlation from Daubert et al.;[18] ▼, correlation from Mokraoui et al.[10]

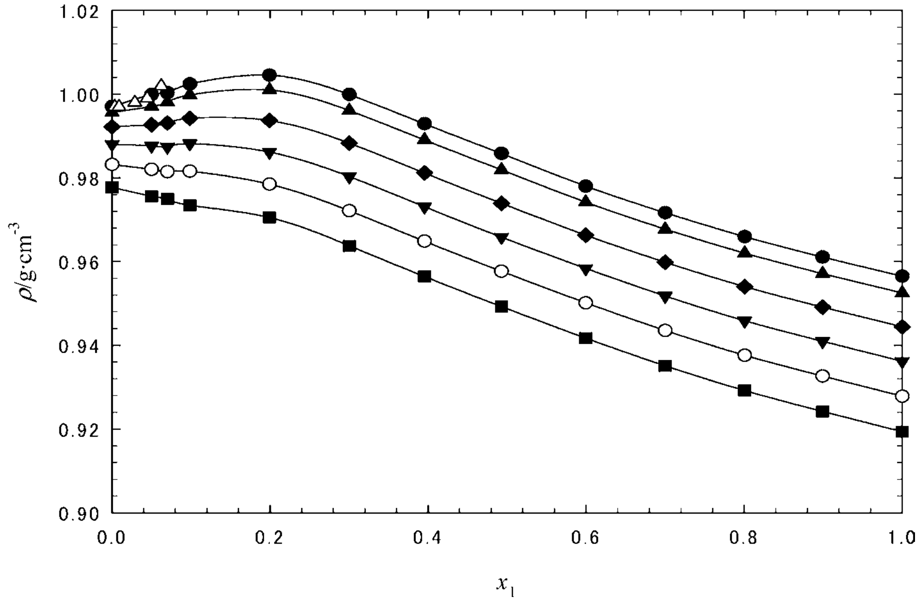

Figure 2. Densities of the 1-AP (1) + water (2) system at: ●, 298.15 K; ▲, 303.15 K; ◆, 313.15 K; ▼, 323.15 K; ○, 333.15 K; ■, 343.15 K; △, Hikita et al.;[9] —, polynomial.

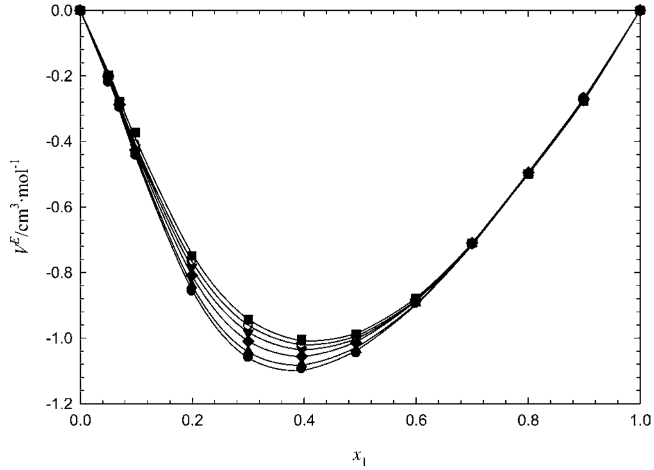

Figure 3. Excess molar volumes of the 1-AP (1) + water (2) system at: ●, 298.15 K; ▲, 303.15 K; ◆, 313.15 K; ▼, 323.15 K; ○, 333.15 K; ■, 343.15 K; —, eq 3.

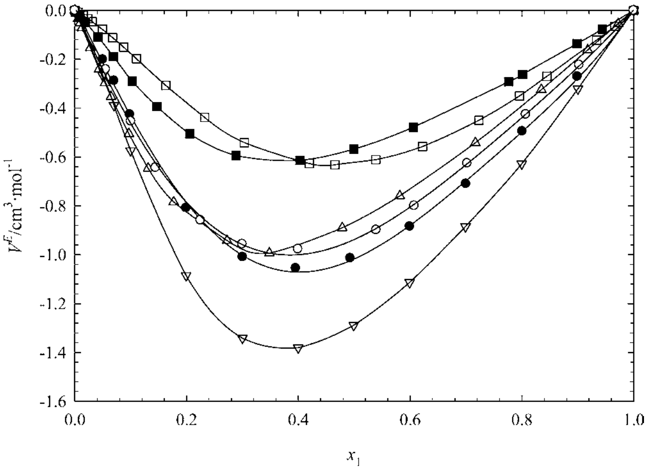

Figure 4. Excess molar volumes of various aqueous alkanolamine systems at 313.15 K: ●, 1-AP; △, TEA;[21] □, MEA;[21] ■, DEA;[21] ▽, AEEA;[20] ○, DGA;[14] —, eq 3.

of 1-AP. As the temperature increases, the effect of the composition on viscosity decreases.

The viscosities of pure 1-AP are well-represented by the Arrhenius equation:

$$\eta/\text{mPa}\cdot\text{s} = A\text{e}^{E/RT} \qquad (6)$$

where A is a system-dependent constant, E is the activation energy for viscous flow, R is the gas constant, and T is temperature. The activation energy value regressed from the data was found to be equal to 38.97 $\text{kJ}\cdot\text{mol}^{-1}$. This value is higher than that of MEA (29.2 $\text{kJ}\cdot\text{mol}^{-1}$)[29] and could be due to stronger hydrogen bonding. The activation energy for flow for 1-AP was closer to the activation energy of that of MDEA (38.0 $\text{kJ}\cdot\text{mol}^{-1}$). Maham et al.[24] reported the activation energies of flow for the mentioned alkanolamines from different sources. Figure 7 displays the different viscosity curves of aqueous solutions of three primary alkanolamines (MEA,[29] 1-AP, and DGA[14]}), two secondary alkanolamines (DEA[30] and AEEA[20]), and a tertiary alkanolamine (MDEA[26]).

Experimental viscosity values of the binary mixtures were used to calculate the viscosity deviation as defined by:

$$\Delta\eta = \eta - \eta_1 x_1 - \eta_2 x_2 \qquad (7)$$

where η is the viscosity of the binary mixture, η_1 and η_2 are those of pure 1-AP and pure water, respectively, and x_1 and x_2 are the mole fractions of the pure components. The viscosity deviation represents deviations from a rectilinear dependence of viscosity on mole fraction. The viscosity deviations ($\Delta\eta$) for 1-AP + water were positive for all of the mole fractions at the temperatures from (298.15 to 343.15) K but were negative for mole fractions close to 0.05 at 298.15 K.

The calculated values of ($Y(x) = \Delta\eta/\text{mPa}\cdot\text{s}$) were correlated with a Redlich−Kister relation as given in eq 3. The coefficients and the standard deviations are presented in Table 4. The *F*-test with a 95 % confidence interval was used to determine the

Table 4. Redlich−Kister Equation Fitting Coefficients of the Derived Properties (V^E, $\Delta\eta$, δn_D, ΔR) for 1-AP (1) + Water (2) Mixtures from (298.15 to 343.15) K

			Excess Volume (V^E/cm^3·mol^{-1})				
T/K	a_0	a_1	a_2	a_3	a_4	a_5	σ/cm^3·mol^{-1}
298.15	−4.125	2.087	−0.943	0.119	1.807	−2.146	0.008
303.15	−4.089	1.930	−0.845	0.604	1.705	−2.709	0.004
313.15	−4.022	1.758	−0.666	0.535	1.372	−2.406	0.003
323.15	−3.989	1.539	−0.432	0.827	1.014	−2.516	0.004
333.15	−3.959	1.410	−0.265	0.782	0.738	−2.290	0.003
343.15	−3.924	1.358	−0.198	0.438	0.794	−1.924	0.001
			Viscosity Deviations ($\Delta\eta$/mPa·s)				
T/K	a_0	a_1	a_2	a_3	a_4		σ/mPa·s
298.15	51.764	20.827	−48.640	13.090	20.759		0.422
303.15	36.598	11.853	−23.187	17.941	7.967		0.272
313.15	21.775	3.672	−11.898	3.689	−7.564		0.512
323.15	13.970	0.836	4.734	8.762	−14.813		0.280
333.15	11.549	0.697	−8.336	4.025	2.636		0.212
343.15	8.018	1.961	0.551	−1.310	−7.860		0.085
			Refractive Index Deviations (δn_D)				
T/K	a_0	a_1	a_2	a_3	a_4	a_5	σ
293.15	0.178	−0.124	0.099	−0.073	−0.018	0.043	0.0002
298.15	0.176	−0.122	0.082	−0.077	0.007	0.051	0.0002
303.15	0.174	−0.119	0.085	−0.071	0.000	0.040	0.0002
308.15	0.171	−0.120	0.082	−0.055	0.004	0.023	0.0003
313.15	0.169	−0.118	0.078	−0.052	0.010	0.020	0.0002
318.15	0.168	−0.120	0.071	−0.045	0.020	0.015	0.0003
323.15	0.166	−0.111	0.085	−0.073	−0.003	0.036	0.0003
328.15	0.167	−0.107	0.066	−0.071	0.018	0.031	0.0002
333.15	0.164	−0.115	0.072	−0.024	0.014	−0.026	0.0003
			Molar Refraction Changes (ΔR/cm^3·mol^{-1})				
T/K	a_0	a_1	a_2	a_3	a_4	a_5	σ/cm^3·mol^{-1}
298.15	−21.727	13.677	−8.075	3.999	−4.974	4.493	0.01
303.15	−21.762	13.727	−7.934	4.263	−5.286	4.118	0.01
313.15	−21.841	13.705	−8.068	4.643	−5.217	3.971	0.01
323.15	−21.921	13.853	−7.846	4.460	−5.825	4.043	0.01
333.15	−21.940	13.796	−8.054	5.186	−5.655	3.327	0.01

optimum number of coefficients. As shown in Figure 8, the viscosity deviations at 313.15 K for aqueous MEA,[29] DGA,[14] AEEA,[20] MDEA,[26] and 1-AP solutions seem to have a change in sign from negative to positive at low alkanolamine concentrations. This is in sharp contrast to the appearance of the viscosity deviation curve for the secondary alkanolamine, DEA.[30]

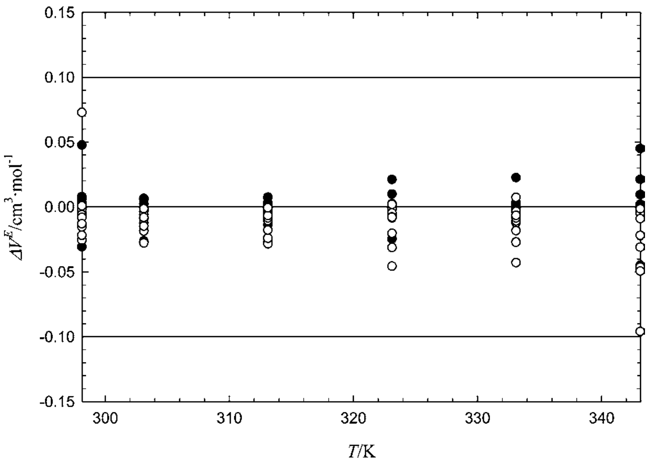

Figure 5. Relative deviations of excess molar volumes of the (1-AP + water) system: ●, relative deviation between experimental data and those calculated from Redlich−Kister coefficients obtained in this work; ○, relative deviation between experimental data and those calculated from Redlich−Kister coefficients obtained from Mokraoui et al.[10]

Table 5. Partial Molar Volumes of 1-AP at Infinite Dilution in Water, V_1^∞, and Water at Infinite Dilution in 1-AP, V_2^∞, from (298.15 to 343.15) K

T K	V_1^∞ cm^3·mol^{-1}	V_2^∞ cm^3·mol^{-1}	V_1^0 cm^3·mol^{-1}	V_2^0 cm^3·mol^{-1}
298.15	75.2	14.9	78.5	18.1
303.15	75.8	14.7	78.9	18.1
313.15	76.3	14.7	79.5	18.2
323.15	77.0	14.7	80.2	18.2
333.15	77.6	14.7	81.0	18.3
343.15	78.5	15.0	81.7	18.4

Experimentally measured refractive indices of the binary solutions of aqueous 1-AP solutions at (293.15 to 333.15) K are listed in Table 3. Figure 9 shows the refractive indices at various temperatures of the aqueous mixture of 1-AP (1) + water (2). There is a sharp increase in the values of the refractive index of the mixture after the addition of 1-AP at all temperatures. The refractive indices deviations δn_D at various temperatures from the linear additive values of the mole fractions are obtained by:

$$\delta n_D = n_D - (x_1 n_{D1} + x_2 n_{D2}) \qquad (8)$$

where n_D is the refractive index of the mixture and n_{D1} and n_{D2} are the refractive indices of the components 1-AP and water, respectively. All values of δn_D were positive for the entire

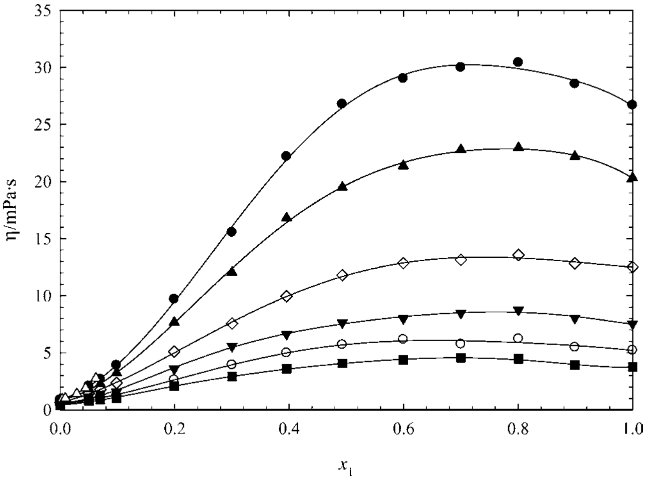

Figure 6. Viscosities of the 1-AP (1) + water (2) system at: ●, 298.15 K; ▲, 303.15 K; ♦, 313.15 K; ◇, 323.15 K; ○, 333.15 K; ■, 343.15 K; △, Hikita et al.;[9] —, polynomial.

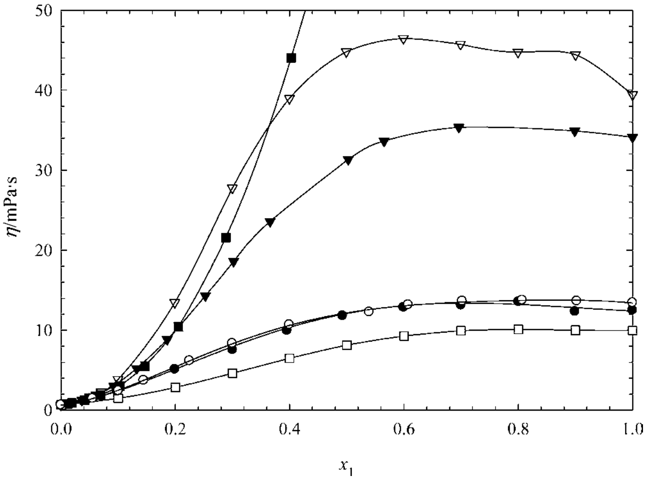

Figure 7. Comparison of the viscosities of various aqueous alkanolamines solutions at 313.15 K: ●, 1-AP; □, MEA;[21] ■, DEA;[21] ▽, AEEA;[20] ○, DGA;[14] ▼, MDEA;[21] —, polynomial.

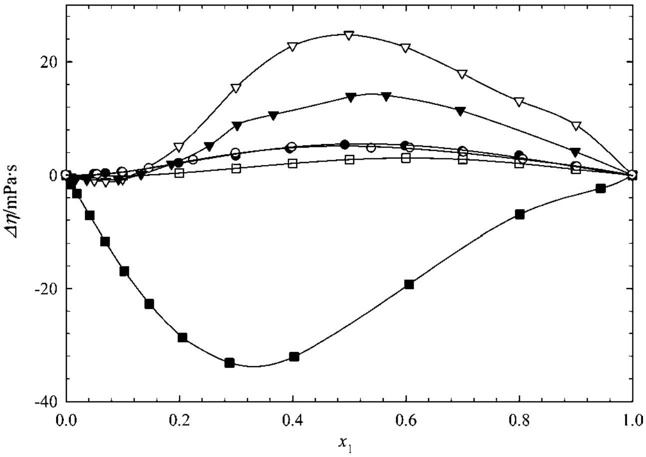

Figure 8. Comparison of the viscosity deviations of various aqueous alkanolamine solutions at 313.15 K: ●, 1-AP; □, MEA;[21] ■, DEA;[21] ▽, AEEA;[20] ○, DGA;[14] ▼, MDEA;[21] —, eq 3.

composition range, and the maximum values of δn_D occurred at $x_1 = 0.3$ at all temperatures.

The calculated values of ($Y(x) = \delta n_D$) were correlated with a Redlich−Kister relation.[11] The coefficients and the standard deviations are presented in Table 4. The *F*-test with a 95 % confidence interval was used to determine the optimum number of coefficients.

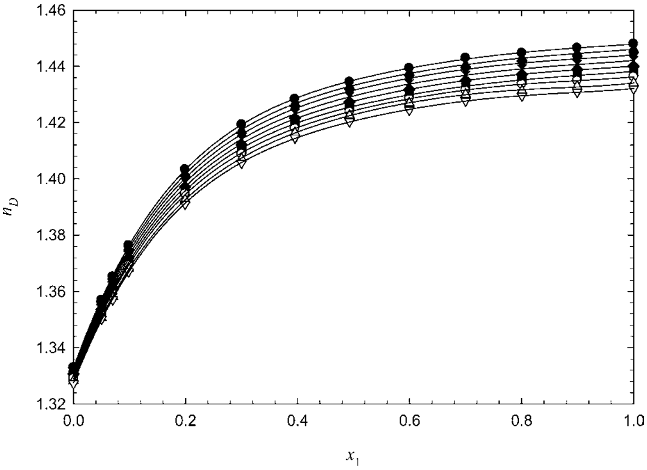

Figure 9. Refractive indices of 1-AP (1) + water (2) system at: ●, 293.15 K; ▲, 298.15 K; ▼, 303 K; ×, 308 K; ◆, 313 K; ■, 318 K; ○, 323 K; △, 328 K; ▽, 333 K; —, polynomial.

Molar refraction changes (ΔR) at various temperatures were calculated from the following relations employing refractive indices and molar volumes.[20] A Redlich−Kister relation given in eq 3 was used to correlate molar refraction changes as a function of mole fraction ($Y(x) = \Delta R$).

$$\Delta R/\mathrm{cm^3 \cdot mol^{-1}} = R - \phi_1 R_1 - \phi_2 R_2 \qquad (9)$$

$$R = \left(\frac{n_D^{\,2} - 1}{n_D^{\,2} + 2}\right)\left(\frac{x_1 M_1 + x_2 M_2}{\rho}\right) \qquad (10)$$

$$R_i = \left(\frac{n_D^{\,i2} - 1}{n_D^{\,i2} + 2}\right)\left(\frac{M_i}{\rho_i}\right) \qquad (11)$$

$$\phi_i = \frac{x_i V_i}{\sum_{i=1}^{2} x_i V_i} \qquad (12)$$

The coefficients and the standard deviations are presented in Table 4. Molar refraction changes were negative for the system studied over the entire range of mole fractions for all five temperatures. ΔR shows negligible temperature dependence with a minimum at $x_1 = 0.3$.

Conclusions

In the present work, the densities and viscosities of the aqueous 1-AP (MIPA) solutions have been measured experimentally over a range of temperature from (298.15 to 343.15) K and refractive indices over a range of temperature from (298.15 to 333.15) K. Excess molar volumes (V^E) values for the aqueous 1-AP solutions calculated from the data were all negative at all temperatures and compositions. The addition of 1-AP to water had no effect on its structure according to the criterion proposed by Hepler,[22] a conclusion similar to that of Maham et al.[21,24] for MEA, DEA, and TEA and Mundhwa et al.[20] for AEEA. Viscosity deviations ($\Delta\eta$) for aqueous 1-AP solutions were all positive for all mole fractions at all temperatures except at a mole fraction of 0.05. The calculated refractive index deviations for the aqueous 1-AP solutions were all positive at all temperatures and compositions. Similar to aqueous AEEA,[20] DGA,[14] MDEA,[26] and MEA[29] solutions, 1-AP exhibited S-shaped viscosity curves and a change in the sign from negative to positive in the water-rich region. Near a mole fraction of 0.8 (4 mol 1-AP to 1 mol of water), there is a possibility of complex formation in solution according to the suggestion by Fort and Moore, which would be in contradiction with Hepler's criteria. Molar refraction changes were negative for 1-AP over the entire range of mole fractions for all temperatures, and at the mole fraction of 0.3, a minimum in ΔR occurred. Changes in molar refraction with respect to temperature were negligible.

Literature Cited

(1) Astarita, G.; Savage, D. W.; Bisio, A. *Gas Treating with Chemical Solvents*; John Wiley & Sons: New York, 1983.

(2) Blauwhoff, P. M. M.; Versteeg, G. F.; Van Swaaij, W. P. M. A study on the reaction between CO_2 and alkanolamines in aqueous solutions. *Chem. Eng. Sci.* **1983**, *9*, 1411–1429.

(3) Camacho, F.; Sanchez, S.; Pacheco, R. Absorption of carbon dioxide at high partial pressures in 1-Amino-2-propanol aqueous solution. Considerations of thermal effects. *Ind. Eng. Chem. Res.* **1997**, *10*, 4358–4364.

(4) Sada, E.; Kumazawa, H.; Butt, M. A. Solubility and diffusivity of gases in aqueous solutions of amines. *J. Chem. Eng. Data* **1978**, *2*, 161–163.

(5) Bavbek, O.; Alper, E. Reaction mechanism and kinetics of aqueous solutions of primary and secondary alkanolamines and carbon dioxide. *Turk. J. Chem.* **1999**, 293–300.

(6) Penny, D. E.; Ritter, E. J. Kinetic study of the reaction between carbon dioxide and primary amines. *J. Chem. Soc., Faraday Trans. 1* **1983**, 2103–2109.

(7) Hikita, H.; Asai, S.; Ishikawa, H.; Honda, M. The kinetics of reactions of carbon dioxide with Monoisopropanolamine, Diglycolamine and Ethylenediamine by a rapid mixing method. *Chem. Eng. J.* **1977**, *14*, 27–30.

(8) Henni, A.; Li, J.; Tontiwachwuthikul, P. Reaction kinetics of CO_2 in Aqueous 1-Amino-2-Propanol, 3-Amino-1-Propanol, and Dimethylmonoethanolamine Solutions in the Temperature Range of 298−313 K Using the Stopped-Flow Technique. *Ind. Eng. Chem. Res.* **2008**, *7*, 2213–2220.

(9) Hikita, H.; Ishikawa, H.; Murakami, E.; Ishii, T. Densities, viscosities and diffusivities of aqueous MIPA, DIPA, DGA and EDA solutions. *J. Chem. Eng. Jpn.* **1981**, *5*, 411–413.

(10) Mokraoui, S.; Valtz, A.; Coquelet, C.; Richon, D. Volumetric properties of the isopropanolamine-water mixture at atmospheric pressure from 283.15 to 353.15 K. *Thermochim. Acta* **2006**, *440*, 122–128.

(11) Bettin, H.; Spieweck, F. The density of water as a function of temperature, after the introduction of International Temperature Scale. *PTB-Mitt.* **1990**, *100*, 195–196.

(12) *Annual Book of ASTM Standards: Density and Relative Density of Liquids By Digital Density Meter*, Standard D 4052-81; American Society of Testing Materials: West Conshohocken, PA, 1986; pp 294−298.

(13) Cannon, M. R.; Manning, R. E.; Bell, J. D. Viscosity Measurement: The kinetic energy correction and a new viscometer. *Anal. Chem.* **1960**, *32*, 355–358.

(14) Henni, A.; Tontiwachwuthikul, P.; Chakma, A.; Mather, A. E. Volumetric properties and viscosities for aqueous Diglycolamine solutions from 25 °C to 70 °C. *J. Chem. Eng. Data* **2001**, *1*, 56–62.

(15) Stokes, R. H.; Mills, R. *Viscosity of Electrolytes and Related Properties*; Pergamon Press: New York, 1965.

(16) Li, J.; Mundhwa, M.; Tontiwachwuthikul, P.; Henni, A. Volumetric properties, viscosities, and refractive indices for aqueous 2-(Methylamino) ethanol solutions from (298.15 to 343.15) K. *J. Chem. Eng. Data* **2007**, *52*, 560–565.

(17) Li, J.; Mundhwa, M.; Henni, A. Volumetric Properties, viscosities, and refractive indices and surface tensions for aqueous Genosorb 1753 solutions. *J. Chem. Eng. Data* **2007**, *52*, 955–958.

(18) Daubert, T. E.; Danner, R. P.; Sibel, H. M.; Stebbins, C. C. *Physical and thermodynamic properties of pure chemicals*; Data Compilation, Taylor & Francis: Washington, DC, 1997.

(19) Pal, A.; Singh, W. Excess molar volumes of linear and cyclic Ethers + Chloroethenes at 298.15 K. *J. Chem. Eng. Data* **1996**, *3*, 428–430.

(20) Mundhwa, M.; Alam, R.; Henni, A. Volumetric properties, viscosities, and refractive indices for aqueous 2-((2-Aminoethyl)amino)ethanol solutions from (298.15 to 343.15) K. *J. Chem. Eng. Data* **2006**, *4*, 1268–1273.

(21) Maham, Y.; Teng, T. T.; Hepler, L. G.; Mather, A. E. Densities, excess molar volumes, and partial molar volumes for binary mixtures of water with monoethanolamine, diethanolamine, and triethanolamine from 25 to 80 °C. *J. Solution Chem.* **1994**, *2*, 195–205.

(22) Hepler, L. G. Thermal expansion and structure in water and aqueous solutions. *Can. J. Chem.* **1969**, 4613–4617.

(23) Neal, J. L.; Goring, D. A. I. Volume-temperature relations of hydrophobic and hydrophilic nonelectrolytes in water. *J. Phys. Chem.* **1970**, *3*, 658–664.

(24) Maham, Y.; Teng, T. T.; Mather, A. E.; Hepler, L. G. Volumetric properties of (Water−Diethanolamine) systems. *Can. J. Chem.* **1995**, 1514–1519.

(25) Zhang, F.; Li, H.; Dai, M.; Zhao, J.; Chao, J. P. Volumetric properties of binary mixtures of water with ethanolamine alkyl derivatives. *Thermochim. Acta* **1995**, 347–357.

(26) Henni, A.; Maham, Y.; Tontiwachwuthikul, P.; Chakma, A.; Mather, A. E. Densities and viscosities for binary mixtures of *N*-Methyldiethanolamine + Triethylene Glycol Monomethyl Ether from 25 °C to 70 °C and *N*-Methyldiethanolamine + Ethanol Mixtures at 40 °C. *J. Chem. Eng. Data* **2000**, *2*, 247–253.

(27) Fort, R. J.; Moore, W. R. Viscosities of binary liquid mixtures. *Trans. Faraday Soc.* **1966**, 1112–1119.

(28) Liler, M.; Kosanović, D. *Hydrogen Bonding of Nitrocompounds with Sulphuric Acid in Hydrogen Bonding*; Pergamon Press: London, 1959; pp 529−543.

(29) Lee, M.; Lin, T. Density and Viscosity for Monoethanolamine + Water, + Ethanol, and + 2-Propanol. *J. Chem. Eng. Data* **1995**, *1*, 336–339.

(30) Teng, T. T.; Maham, Y.; Hepler, L. G.; Mather, A. E. Viscosity of aqueous solutions of *N*-Methyldiethanolamine and of Diethanolamine. *J. Chem. Eng. Data* **1994**, *2*, 290–293.

Received for review March 26, 2010. Accepted October 13, 2010. The financial support of the Natural Sciences and Engineering Research Council of Canada (NSERC), the Natural Resources Canada (NRCan), the Canadian Foundation for Innovation (CFI), the Petroleum Technology Research Centre (PTRC), and the International Test Center for Carbon Dioxide Capture (ITC, University of Regina) are gratefully acknowledged.

JE100300S