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Physicochemical properties of alkanolamine-choline chloride deep eutectic solvents: Measurements, group contribution and artificial intelligence prediction techniques

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ABSTRACT

Further development in the utilization of deep eutectic solvents (DESs) for new processes requires an insightful understanding of their fundamental properties. Hence, in this study, we report experimental measurements of the density, viscosity, conductivity, pH, surface tension and thermal stability of three different amine based deep eutectic solvents (DESs), (Choline chloride + monoethanolamine, ChCl-MEA), (Choline chloride + diethanolamine, ChCl-DEA) and (Choline chloride + methyldiethanolamine, ChCl-MDEA), representing the primary, secondary and tertiary amines, respectively. The experimental data was obtained at temperature from 293.15–353.15 K and for three different choline chloride to amine molar ratios of 1:6, 1:8 and 1:10. Moreover, the densities of the amine based DESs were predicted with the empirical group contribution method, conventional artificial neural network (ANN) and bagging artificial neural network (ANN). Due to the special nature of bonds that exists between the alkanol-amines and the choline chloride salt, the deviations for the traditional group contribution and ANN methods are quite high when compared to the experimental values. Hence, a technique based on bagging ANN, which combines the results of several ANNs in order to reduce the deviations and errors, was established. The experimental results revealed that amine-based DESs are more thermally stable as compared to stand-alone amine solvents. The density, viscosity, stability and conductivity increased with decreasing choline chloride to amine molar ratio in the DESs. However, there was no clear trend in the pH with molar ratio. The bagging ANN provided the best prediction for both the density and conductivity of the amine based DESs with a normalized mean square error (NMSE) of 2.799×10^{-7} and 5.820×10^{-4}, respectively.
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1. Introduction

Since its inception [1], deep eutectic solvents (DESs) had gained significant attention due to their better characteristics coupled with their applicability in various fields including electrochemistry, nanomaterials, biochemistry, synthesis, separation and analysis. The emergence of DESs was engendered out of the urgent necessity to eliminate the limitations encountered from conventional solvents and ionic liquids (ILs) such as toxicity, high cost, poor degradability and other environmental concerns. In addition to their benefits over ILs, DESs are often cheap, simple to prepare, less toxic and biodegradable. For example, Choline chloride (Vitamin B4), the salt used for the preparation of DESs in this study, is quite cheap, non- toxic and biodegradable.

However, further developments in the utilization of DESs require an insightful understanding of their fundamental properties. Although there have been significant studies on the experimental determination of the physicochemical properties of DESs such as density, viscosity, surface tension, conductivity, pH etc. [2–11], data obtained on the physicochemical properties of many DESs are often incomplete and insufficient [12]. Consequently, the prediction of the physicochemical properties of deep eutectic solvents is gaining great attention because the determination of these properties through experiments can be time consuming, expensive, difficult or impossible at all temperatures and pressures. Amongst the top predictive techniques that have been the focus of recent studies are the group contribution and artificial intelligence methods [13–15]. One of the studies reported the prediction of the density of conventional DESs from temperatures ranging from 298.15–368.15 K using the modified Rackett method [13]. However, their study did not include any amine based DES. Shahbaz et al. [14] worked on the prediction of the density of ammonium and phosphonium based DESs using glycerol and ethylene glycol as the hydrogen bond donors (HBDs) using the modified Rackett and traditional artificial neural network (ANN) methods. Bagh et al. [15] conducted the determination of the electrical conductivity of some ammonium and phosphonium based DESs using traditional ANN. However, the conventional ANN and group contribution methods produced results with low accuracy. A new means of achieving high accuracy for the prediction of

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physicochemical properties of DESs becomes crucial. One of these methods is the bagging ANN technique, which is based on aggregating the outputs from several conventional ANN in order to reduce the deviations.

In this study, we report experimental measurements of the density, viscosity, conductivity, pH, surface tension and thermal stability of three different amine based deep eutectic solvents, ChCl-MEA, ChCl-DEA, and ChCl-MDEA representing the primary, secondary and tertiary amines, respectively. The three amine based deep eutectic solvents have been carefully selected based on their CO_2 absorption capacity, feasibility of forming a miscible eutectic mixture during the preparation stage and their potentiality for applications in carbon capture purposes. The experimental data was obtained at temperature from 293.15–353.15 K and for three different ChCl to amine molar ratios of 1:6, 1:8 and 1:10. In addition, predictions based on the group contribution (the modified Rackett method), conventional ANN and bagging ANN were conducted for the density and conductivity.

2. Experimental

2.1. Materials

Monoethanolamine (MEA), diethanolamine (DEA), methyldiethanolamine (MDEA), acetone, deionized water, ethylene glycol, glycerol and choline chloride (2-hydroxyethyltrimethylammonium) were all purchased from Sigma Aldrich (USA), Purite (UK) and BDH (UK) chemicals. All materials were used without any further purification because of its prior purity level. Detailed information about each chemical is provided in Table 1.

2.2. DES Preparation

In this work, the method of preparation reported in previous study was used [1]. The proper quantities of salt and HBD were put in a well-sealed vial. The mixture was vigorously shaken at 90 °C until a homogeneous liquid is obtained. Thereafter, the mixture was left to cool down to room temperature. If the mixture is in the liquid phase and no precipitate appears for a few days, then the DESs is used for further investigations.

2.3. Freezing point

The freezing point of the samples were measured with Perkin Elmer Differential Scanning Calorimeter 4000 (UK) because it offers dependable performance and quality results. In addition, it has a wide temperature range from −120 °C to 725 °C with a repeatability of ±0.1 °C. The equipment was calibrated with Indium during installation. In addition, the equipment was tested using solvents with known freezing points such as water and monoethanolamine.

2.4. Density

The density of the samples was measured using Anton Paar DMA 5000 M density meter (Austria/Europe). The density meter 5000 M was selected because it can measure density in the wide range of 0–3 g/cm^3 and temperature in the range of 0–100 °C. Moreover, the density accuracy and precision are 5 μg/cm^3 and 1 μg/cm^3 respectively which are decent for this experiment. The equipment was tested using ChCl-Glycerol and ChCl-Ethylene glycol DESs.

2.5. Viscosity

The viscosities of the samples were obtained using Thermo Scientific Haake Rheostress Mars Technologies 6000 rheometer because of its temperature range of −80–500 °C. The equipment was tested with ChCl-Glycerol and ChCl-Ethylene glycol DESs.

2.6. pH

The pH measurements were obtained using Delta Ohm's HD 22569.2 meter because it has a measuring range from −9.999 to +19.999. In addition, it has a resolution of 0.001 pH and an accuracy of ±0.001. The pH meter was tested with three buffers of known pH 10, 7 and 4. The measured values compared well with the labeled values.

2.7. Conductivity

The conductivity of the DESs was obtained with SciChem Tech SCT-CADY conductivity meter because it has a measuring range of conductivity of 0–200 mS/cm. In addition, the meter has a resolution of 0.01 mS/cm and an accuracy of 1.0%. The meter was tested with a standard solution of 1413 μS/cm. The electrode or probe was rinsed with deionized water between different measurements to prevent cross contamination.

2.8. Surface tension

The surface tension was measured by Kruss GmbH Drop Shape Analyzer DSA25 because it has resolution and accuracy of 0.01 mN/m and 0.3 mN/m respectively. The equipment was tested using samples of water, acetone and monoethanolamine (MEA). The results compared well with the reported values in the literature.

3. Properties prediction methods

3.1. Group contribution method

The modified Rackett method was utilized for the prediction of the density of the alkanolamine-choline chloride DESs. The estimation starts with the determination of the critical properties of the individual salt and hydrogen bond donors with the Modified Lydersen–Joback–Reid method suggested by Alvarez and Valderrama [16].

$$T_b = 198.2 + \sum n\Delta T_{bM} \tag{1}$$

$$T_c = \frac{T_b}{\left[A_M + B_M \sum n\Delta T_M - \left(\sum n\Delta T_M\right)^2\right]} \tag{2}$$

$$P_c = \frac{M}{\left(C_M + \sum n\Delta P_M\right)^2} \tag{3}$$

$$V_c = E_M + \sum n\Delta V_M \tag{4}$$

Table 1
Source and purity of all materials used.

Parameters\Compound	Choline Chloride	MEA	DEA	MDEA	DI Water	Acetone	Ethylene Glycol	Glycerol
Source	Sigma Aldrich (US)	Sigma Aldrich (US)	Sigma Aldrich (US)	Sigma Aldrich (US)	Purite (UK)	Sigma Aldrich (US)	BDH (UK)	Sigma Aldrich (US)
Purity	≥98.0%	≥99.0%	≥98.0%	≥99.0%	≥99.9%	≥99.9%	≥99.0%	≥99.5%
Water Content	N/A	≤0.30%	≤0.20%	≤0.30%	N/A	≤0.50%	≤0.20%	≤0.10%

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