Fluid Phase Equilibria 557 (2022) 113435

Contents lists available at ScienceDirect

Fluid Phase Equilibria

journal homepage: www.elsevier.com/locate/fluid

Thermophysical characterization of choline chloride: Resorcinol and its mixtures with water

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ARTICLE INFO

Article history:
Received 29 December 2021
Revised 18 February 2022
Accepted 28 February 2022
Available online 1 March 2022

Keywords:
Physicochemical properties
Choline chloride:resorcinol

ABSTRACT

The study of deep eutectic solvents has increased in recent years. This is because of their great solubility ability and lower toxicity than usual organic solvents. In this work, deep eutectic solvents formed by choline chloride and resorcinol in the mole ratio 1:2 and its mixtures with water, e.g., choline chloride:resorcinol:water 1:2:1.05 (water mass fraction = 0.05) and choline chloride:resorcinol:water 1:2:2.22 (water mass fraction = 0.1), have been studied. Several physicochemical properties (density, speed of sound, isentropic compressibility, refractive index, surface tension, isobaric molar heat capacity, viscosity, and electrical conductivity) have been obtained and analysed at atmospheric pressure in the range of 283.15–338.15 K. The starting temperature for the speed of sound measurements was 308.15 K. The effects of temperature and water inclusion have been evaluated. The obtained results have shown a linear correlation between density, speed of sound, refractive index, surface tension and isobaric molar heat capacity and temperature. Additionally, the viscosity and electrical conductivity data can be adjusted using the Vogel-Fulcher-Tammann equation. Finally, the inclusion of water was analysed to check how the thermophysical properties were modified. These modifications had greater effects on transport properties, viscosity and electrical conductivity.

1. Introduction

Scientists are making real efforts to find new solvents that can be considered green solvents but also present good properties for industrial applications. Some of these properties are related to recyclability, selectivity, melting point, flammability, corrosivity, and solubility, amongst others [1,2].

Several families, such as ionic liquids (ILs), supercritical solvents or even solvents from biomass, have been proposed as alternatives to traditional solvents [3,4]. In recent decades, deep eutectic solvents (DESs) have emerged as a new family of green solvents because of their environmental and health properties, low cost and biodegradability.

DESs are mixtures formed by two or more compounds melting at lower temperatures than the ideal liquid mixture [5]. DESs are combinations of one or more hydrogen bond acceptors (HBAs) and hydrogen bond donors (HBDs).

Many studies show the potential applications of DESs: these mixtures can be used in synthesis and separation processes [6,7], extraction [8–11], biocatalysis [12,13], biomedical applications [14,15], electrochemistry [16,17], biofuels [18], or in the pharmaceutical industry [19–22].

The particular physicochemical properties of DESs have drawn the attention of the scientific community. They present low vapour pressure and volatility, nonflammability, and chemical and thermal stability, as well as being compatible with water and environmentally friendly. All of these properties are reflections of the strong hydrogen-bonding interactions [23] formed within their structure.

In this work, we chose choline chloride (ChCl) as the HBA and resorcinol as the HBD to form a DES. ChCl is a typical substance used for the formation of DESs, and resorcinol has been widely studied because of its pharmaceutical properties. For instance, it is used topically for its antiseptic, antifungal, antipruritic, exfoliative and keratolytic properties [24]. Carriazo et al. previously studied several DESs formed by resorcinol and used them in the synthesis of hierarchical porous carbon monoliths as carbonaceous pre-

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https://doi.org/10.1016/j.fluid.2022.113435

Table 1
Chemical information.

Chemical name	CAS No	Source	Mass fraction purity[a]	Molar mass/g·mol^{-1}
Choline chloride	67–48–1	Sigma	0.998	139.624
Resorcinol	108–46–3	Sigma-Aldrich	0.999	110.1106

[a] As stated by the supplier.

cursors and templating agents [25]. Woo et al. prepared a weakly acidic DES formed by ChCl and resorcinol to explore its extraction of lignocellulosic materials; however, they observed that alkali DES extract was better than acidic DES [26]. Other DESs formed with imidazole and resorcinol (1:1) have been used for the efficient capture of NH_3 [27].

We prepared DES with choline chloride and resorcinol in a 1:2 mole ratio. The chosen composition allows thermophysical characterization in the desired temperature range. On the other hand, it is a mole ratio that is commonly studied in a large number of choline chloride-based DESs. Furthermore, we characterized two of its mixtures with water:choline chloride:resorcinol:water 1:2:1.05 (water mass fraction = 0.05) and choline chloride:resorcinol:water 1:2:2.22 (water mass fraction = 0.1) to study the effect of dilution on the thermophysical properties of choline chloride-resorcinol. This eutectic system containing resorcinol could have interest in the pharmaceutical field when used in liquid formulations.

Once the DES was prepared, its molecular structure was studied through NMR techniques. The thermophysical characterization at $p = 0.1$ MPa was used to obtain the following properties: density, refractive index, surface tension, isobaric molar heat capacity, viscosity, and electrical conductivity in the range of 283.15–338.15 K. The speeds of sound of the studied systems were measured in the temperature range of 303.15–338.15 K due to the ultrasound absorption of these systems [28]. From the experimental data, some interesting, derived properties were calculated. Finally, we also studied the inclusion of water with the objective of analysing the variation in the properties.

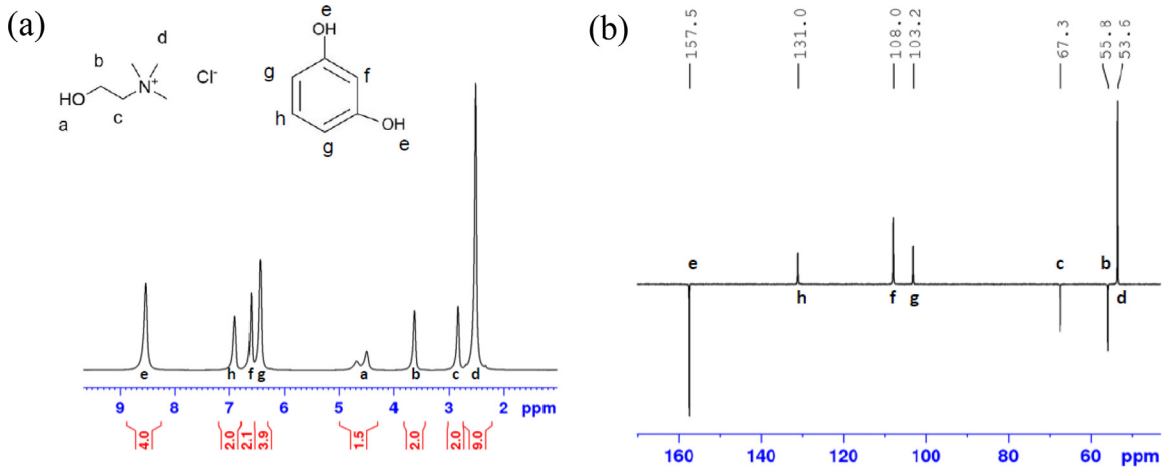

Fig. 1. (a) ^{1}H-RMN and (b) ^{13}C-RMN-APT spectra of the choline chloride:resorcinol (1:2).

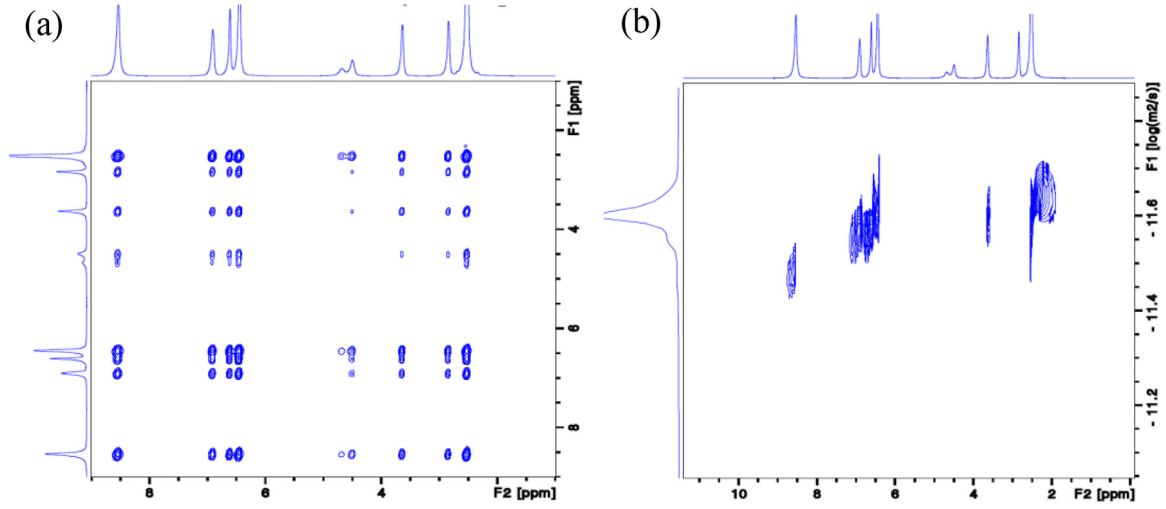

Fig. 2. (a) NOESY and (b) DOSY spectra of the choline chloride:resorcinol (1:2).

2. Materials and methods

2.1. Materials

Table 1 summarizes the information about the compounds used in this study. The low-melting mixture choline chloride + resorcinol (1:2) was prepared by mass employing a Sartorius semimicro balance CP225-D with an uncertainty of $1{\cdot}10^{-5}$ g. The estimated uncertainty in the mole fraction of the DES was 0.01. The final water content of the mixture (350 ppm) was obtained by the Karl Fisher Method using an Automatic Titrator Crison KF 1S-2B On the other hand, the ternary aqueous mixtures were prepared using Milli Pore Milli-Q water with a resistivity of 18.2 MΩ·cm.

2.2. Methods

2.2.1. NMR measurements

NMR experiments were performed using a Bruker AVANCE operating at 400 MHz for ^{1}H. The spectra were obtained at 298.15 K. All shifts have been referenced to TMS, which has been used as an external standard. ^{1}H NMR spectra were recorded with a standard one-pulse sequence with 90 flip angles for excitation, a spectral width of 16 ppm centred at 5 ppm, 16 K data points and a relaxation time fixed to 30 s. Eight scans were acquired for the spectrum. In the case of ^{13}C, NMR spectra were recorded with an APT sequence (Bruker pulse program jmod), with a spectral width of 240 ppm centred at 110 ppm, 64 K data points and relaxation time fixed to 2 s. A total of 256 scans were acquired for each spectrum. COSY, HSQC and HMBC techniques with several Brucker pulse programs (*cosygpmfqf, hsqcedetgp* and *hmbclpndqf,* respectively) were used for signal assignment. The NOESY spectrum (Bruker pulse program *noesygpph*) was obtained with a spectral width of 4 ppm centred at 4 ppm, 128 t1 increments and 8 scans. Finally, DOSY experiments (Brucker pulse program *stebpgp1 s)* were carried out with a spectral width of 16 ppm centred at 5 ppm and 16 K data points.

2.2.2. Thermophysical properties

Several thermophysical properties have been obtained, including density, speed of sound, isentropic compressibility, refrac-

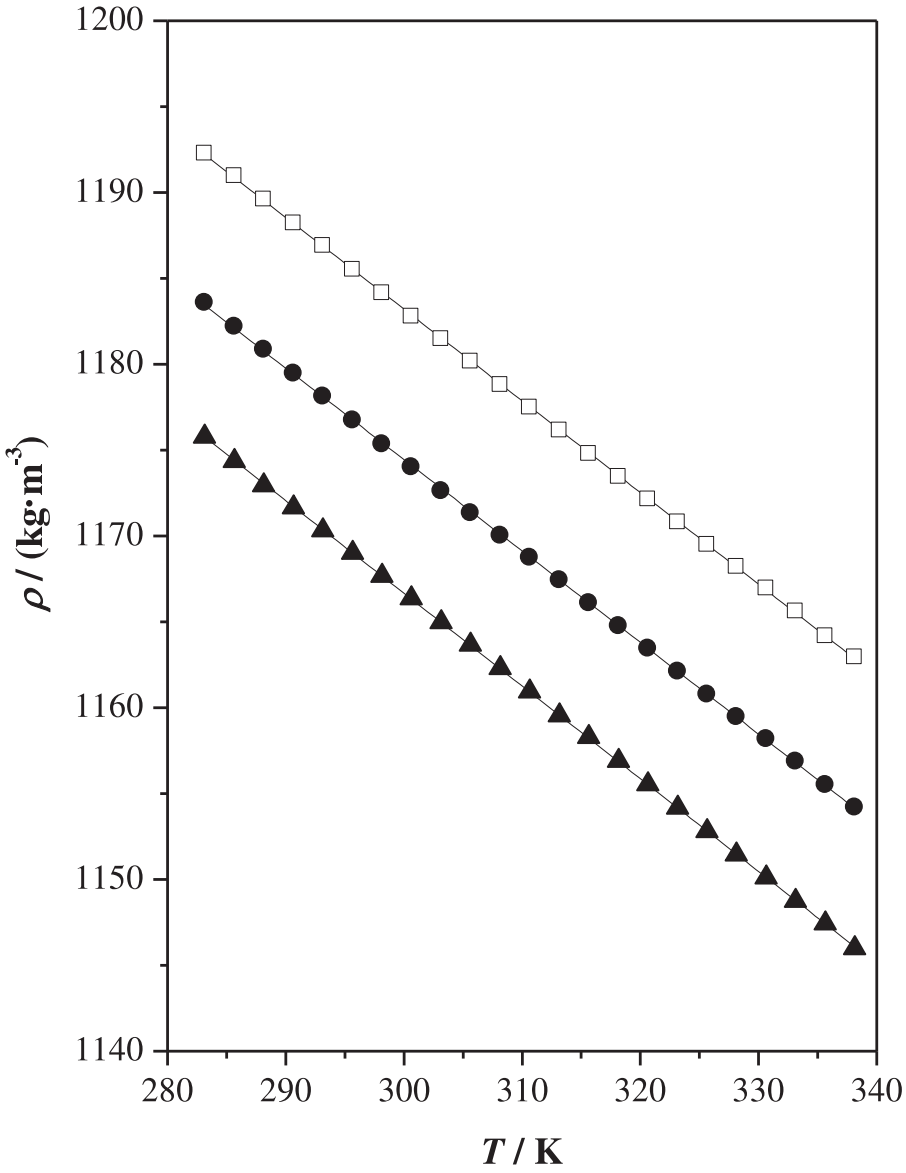

Fig. 3. Density, ρ, as a function of temperature, T, at p = 0.1 MPa for the studied systems: choline chloride:resorcinol (1:2) (□); choline chloride:resorcinol:water (1:2:1.05) (●); choline chloride:resorcinol:water (1:2:2.22) (▲); (—) correlated values.

tive index, surface tension, isobaric molar heat capacity, viscosity, and electrical conductivity. All the measurements were carried out in the temperature range of 283.15–338.15 K at 2.5 K intervals.

Three measurements were made for each property and for each system, and then the results were averaged. Nevertheless, the repeatability of the measurements is lower than the uncertainty; therefore, the deviations amongst measurements are negligible.

Density values, ρ, and speed of sound, u, were obtained simultaneously using an Anton Paar DSA 5000 vibrating tube densimeter and sound analyser (working at 3 MHz). Temperature was controlled internally, with an uncertainty of 0.005 K. The calibration was carried out using dry air and ultrapure water supplied by SH Calibration Service GmbH. The uncertainty of density is 0.1 $kg{\cdot}m^{-3}$ and 0.5 $m{\cdot}s^{-1}$ for speed of sound.

Refractive indices at 589.3 nm sodium D wavelength, n_D, were measured with a digital Abbe Refractometer Zuzi WAY-1S with an external Lauda E-200 thermostat that keeps the temperature constant. The refractive index and temperature uncertainties are 10^{-3} and 0.01 K, respectively.

Surface tensions, σ, were obtained with a drop volume tensiometer, Lauda TVT-2. A thermostat, model Lauda E-200, was used to control the temperature of the sample, with the uncertainty at 0.01 K. The uncertainty for this property is 0.5 $mN{\cdot}m^{-1}$.

Isobaric molar heat capacities, $C_{p,m}$, were determined using a differential scanning TA Instruments Q2000. Synthetic sapphire samples were used as standard references to obtain adequate values. The corresponding uncertainties are 1% for isobaric molar heat capacity and 0.005 K for temperature

In the case of kinematic viscosities, ν, have been determined using a Schoot-GeräteAVS-440 automatic measuring unit along with several Ubbelohde capillary viscosimeters. The uncertainty of the time flow measurements is 0.01 s, and kinetic energy corrections have been applied to the experimental data. The temperature was controlled by means of a Schoot-Geräte CT 1150/2 thermostat, with a temperature uncertainty of 0.01 K. Dynamic viscosity, η, has been obtained from density and kinematic viscosity; the estimated uncertainty for both kinematic and dynamic viscosities is 1%.

Finally, electrical conductivities, κ, were measured using a conductimeter from CRISON, model GLP31, which operates at alternat-

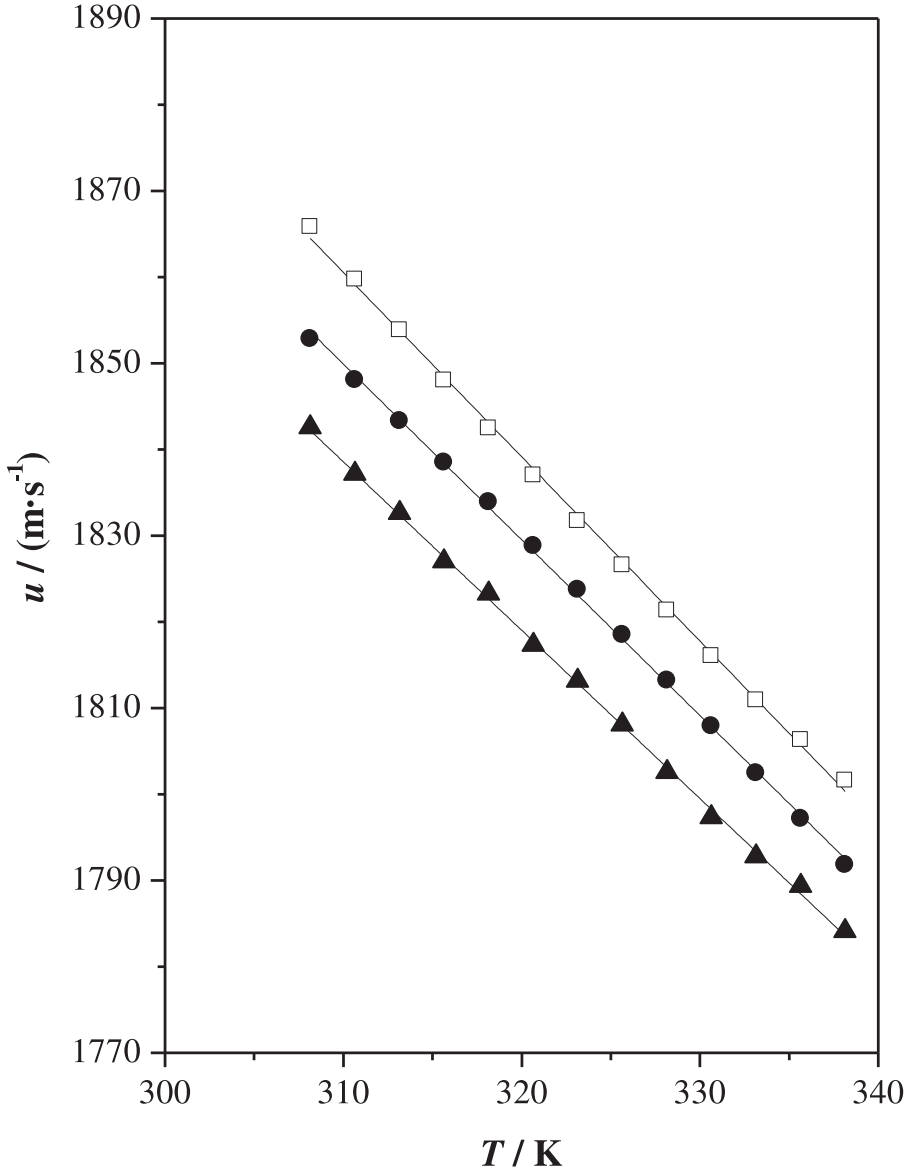

Fig. 4. Speed of sound, u, as a function of temperature, T, at p = 0.1 MPa for the studied systems: choline chloride:resorcinol (1:2) (□); choline chloride:resorcinol:water (1:2:1.05) (●); choline chloride:resorcinol:water (1:2:2.22) (▲); (—) correlated values.

ing frequencies (2 kHz). The temperature of the samples was thermostated to ±0.01 K by means of a Schoot-Geräte CT 1150/2 thermostat. The conductivity cell was calibrated using KCl aqueous solutions supplied by CRISON. The uncertainty of the measurements is 1%.

3. Results and discussion

3.1. NMR characterization

The chemical structure of ChCl:resorcinol (1:2), which was synthetized in this work, was analysed through NMR spectroscopy. The ^{1}H and ^{13}C spectra allowed the identification of the atoms present in the structure. These spectra are shown in Fig. 1. The chemical shifts in ppm at $T = 298.15$ K, are the following: ^{1}H NMR: δ = 2.5 (s, 9H, H_d), 2.8 (s, 2H, H_c), 3.6 (s, 2H, H_b), 4.5 (s, OH, H_a), 6.4 (s, 4H, H_g), 6.6 (s, 2H, H_f), 6.9 (s, 2H, H_h), 8.6 (s, 4H, H_e); ^{13}C δ = 53.6 (t, J = 30 Hz, C_d), 55.8 (C_b), 67.3 (C_c), 103.2 (C_g), 108.0 (C_f), 131 (C_h), 157.5 (C_e). The analysis of the peaks confirmed the mole ratio of the mixture.

The hydrogen coupling through space can be studied with the NOESY technique. Cross peaks indicate inter- or intramolecular interactions, and the positive or negative sign is related to the fast or slow tumbling molecules, respectively. In the studied mixture, negative NOE signals amongst almost all protons (mobile and aliphatic) of both compounds were observed (Fig. 2a). The most intense peaks were those between the hydroxyls of resorcinol and the methyl ones of choline. On the other hand, the interactions of the mobile hydrogen of choline with the rest were weaker. The DOSY spectrum showed four differentiated traces (Fig. 2b); no OH-choline signal was observed. Except for the faster resorcinol hydroxyls, the rest of the hydrogens moved together. All NMR results indicated the presence of a supramolecular structure in the eutectic mixture. This fact agrees with our previous studies for other hydrophilic NADESs [29–31].

3.2. Thermophysical properties

In this paper, several properties have been obtained and analysed in terms of the chemical structure of DES ChCl:resorcinol

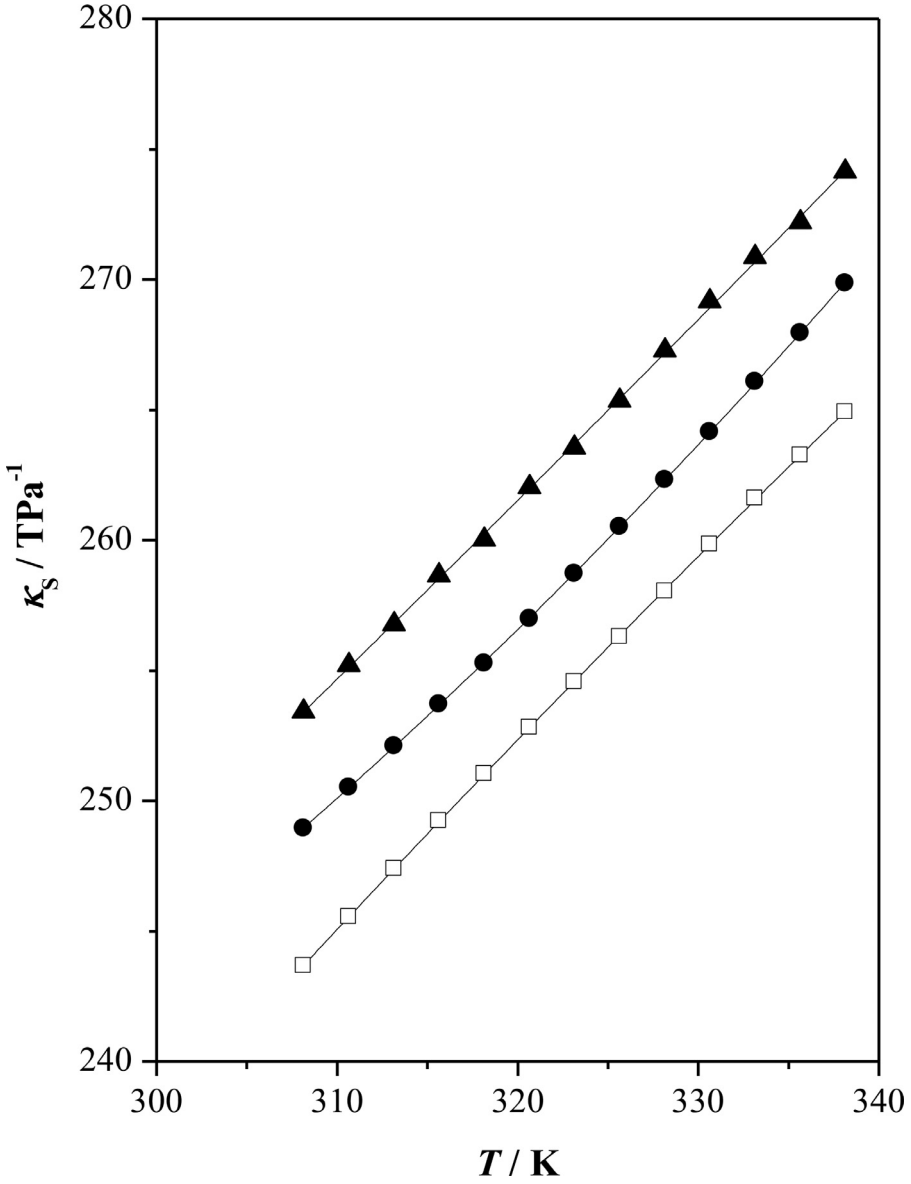

Fig. 5. Isentropic compressibility, κ_S, as a function of temperature, T, at p = 0.1 MPa for the studied systems: choline chloride:resorcinol (1:2) (□); choline chloride:resorcinol:water (1:2:1.05) (●); choline chloride:resorcinol:water (1:2:2.22) (▲); (—) correlated values.

(1:2) and its mixtures with water:choline chloride:resorcinol:water 1:2:1.05 and choline chloride:resorcinol:water 1:2:2.22. Experimental data of density, ρ; speed of sound, u; isentropic compressibility, κ_S; refractive index, n_D; surface tension, σ; isobaric molar heat capacity, $C_{p,m}$; kinematic and dynamic viscosities, ν and η, respectively; and electrical conductivity, κ, are gathered in Table S1 of the Supplementary material and shown in Figs. 3–10.

A linear dependence on temperature has been observed for density, speed of sound, refractive index, surface tension and isobaric molar heat capacity. The experimental data have been correlated with the following equation:

$$Y = AT + B \tag{1}$$

where Y is the studied property and A and B are adjustable parameters. The best linear fitting parameters and relative root-mean square deviations, *RMSDr*, between experimental and correlated values are gathered in Table 2.

$$RMSD_r/\% = 100\left(\frac{1}{n}\sum_{i=1}^{n}\left(\frac{Y_i^{exp} - Y_i^{corr}}{Y_i^{exp}}\right)^2\right)^{1/2} \tag{2}$$

In this study, the experimental values for density decrease as the temperature increases. As with other published DESs, these mixtures present density values higher than water in the range of 1000–1300 kg·m^{-3} [32]. For the studied DES, the values of this property at T = 298.15 K are 1184.15 kg·m^{-3} for ChCl:resorcinol (1:2), 1175.35 kg·m^{-3} for ChCl:resorcinol:water (1:2:1.05), and 1167.68 kg·m^{-3} for ChCl:resorcinol:water (1:2:2.22). It is known that this property can vary with mole ratios and properties of components, as we can see in our obtained results [33].

The average space amongst molecules will be lower at low temperature, so the molar volume will be reduced, and the density will increase. However, this behaviour should be analysed in each

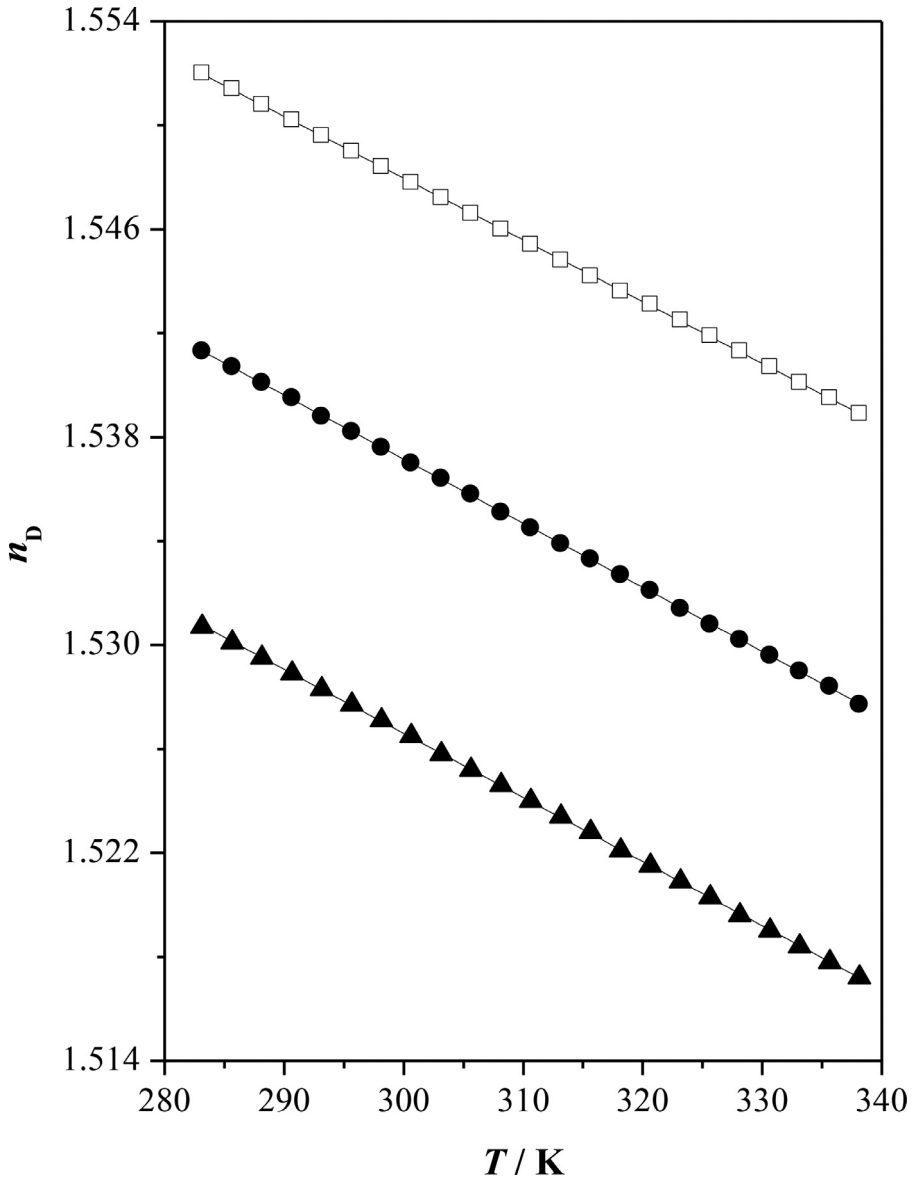

Fig. 6. Refractive index, n_D, as a function of temperature, T, at p = 0.1 MPa for the studied systems: choline chloride:resorcinol (1:2) (□); choline chloride:resorcinol:water (1:2:1.05) (●); choline chloride:resorcinol:water (1:2:2.22) (▲); (—) correlated values.

DES and, especially, when water is included because density values can be modified. In this case, the density decreases as the water content increases. This means that the denser compound is ChCl:resorcinol (1:2), followed by choline ChCl:resorcinol:water (1:2:1.05) and ChCl:resorcinol:water (1:2:2.22). This phenomenon can be related to the molecular organization and the interactions between components. In this sense, density values decrease 0.74% and 1.4% when water is included. These reductions of this property agree with Agieienko et al., who noticed that the density decreases slightly with the content of water [34].

Higher values of speed of sound are found for ChCl:resorcinol (1:2), followed by ChCl:resorcinol:water (1:2:1.05) and ChCl:resorcinol:water (1:2:2.22). The speed of sound of the mixture without water is higher than that of the mixtures with water, with this difference being higher at low temperatures. This property is related to the efficiency in molecular packing, presenting higher speed of sound values when the packing is more effective. In this sense, water inclusion leads to a diminution of this property because the packing is poor. Values decrease with temperature because of the diminution in the ability to transmit the speed of sound decreases. These results can be observed in other published papers [35,36].

The isotropic compressibility, κ_S, can be obtained through the density and speed of sound values with the following equation: $\kappa_S = 1/\rho \cdot u^2$. This equation assumes that the ultrasonic absorption is negligible. This property gives information about the internal organization of the compound structure. Lower isentropic compressibility values are a consequence of more packed structures. For the studied DES, values at $T = 303.15$ K are 240.05 TPa^{-1}, 245.87 TPa^{-1} and 250.45 TPa^{-1} for ChCl:resorcinol (1:2), ChCl:resorcinol:water (1:2:1.05) and ChCl:resorcinol:water (1:2:2.22), respectively. These values indicate that the DES without water is more packed than the others.

The refractive index is defined as the ratio of the velocity of light at a specified wavelength in air to its velocity in the examined chemical. A linear correlation between temperature and

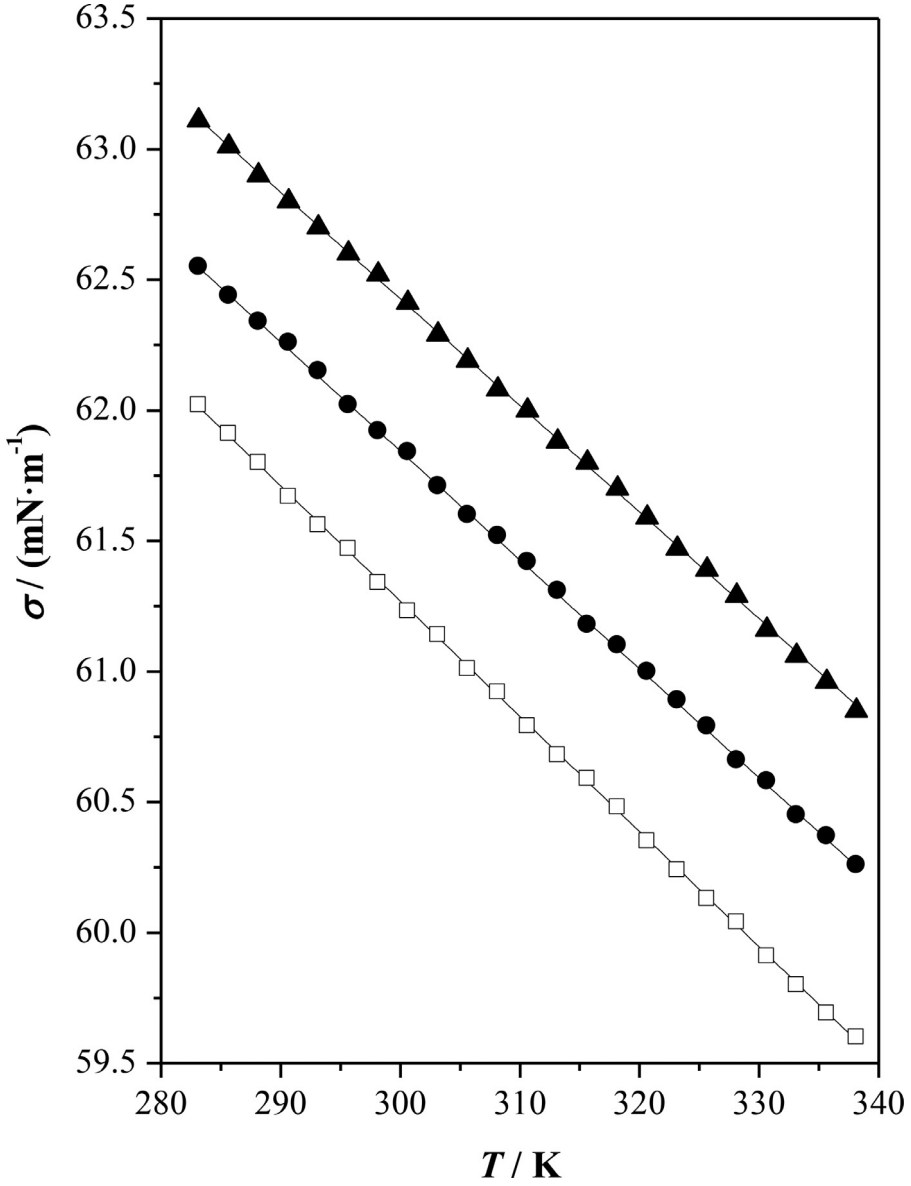

Fig. 7. Surface tension, σ, as a function of temperature, T, at $p = 0.1$ MPa for the studied systems: choline chloride:resorcinol (1:2) (□); choline chloride:resorcinol:water (1:2:1.05) (●); choline chloride:resorcinol:water (1:2:2.22) (▲); (—) correlated values.

refraction index, n_D, has been obtained with higher values at lower temperatures. In this case, the highest values are found for ChCl:resorcinol (1:2), followed by ChCl:resorcinol:water (1:2:1.05) and ChCl:resorcinol:water (1:2:2.22). Additionally, when water is included, this property is modified, obtaining values of 1.5484 for ChCl:resorcinol (1:2), 1.5376 for ChCl:resorcinol:water (1:2:1.05) and 1.5271 for ChCl:resorcinol:water (1:2:2.22) at $T = 298.15$ K, i.e., The higher the content of water is, the lower the refractive index.

The surface tension, σ, depends on the intermolecular forces acting in the bulk phase. Surface tension decreases because of the diminution in these forces with temperature. That is, higher surface tension values are found when stronger intermolecular forces are present. For the studied DES, the surface tension values are relatively high because of the hydrogen bonds formed between choline chloride and resorcinol. In all cases, this property decreases linearly with temperature. For this property, the values found at $T = 298.15$ K, are 61.34 mN·m^{-1} for ChCl:resorcinol (1:2), 61.92 mN·m^{-1} for ChCl:resorcinol:water (1:2:1.05) and 62.52 mN·m^{-1} for ChCl:resorcinol:water (1:2:2.22).

For the isobaric molar heat capacity, $C_{p,m}$, higher values are found for ChCl:resorcinol (1:2) than for ChCl:resorcinol:water (1:2:1.05) and ChCl:resorcinol:water (1:2:2.22). For these mixtures, their values increase with temperature in a linear way. These results are in accordance with other DES published by Zhu et al., who observed that this property changes linearly with temperature [37].

The fluidity and ionicity of ChCl:resorcinol and its mixtures have been measured through kinematic viscosity, ν, and electrical conductivity. Using density values, the dynamic viscosity η was obtained with the following relationship: $\eta = \rho \cdot \nu$.

For these two transport properties, the experimental values can be fitted to a Vogel-Fulcher-Tammann equation [38–40]:

$$\eta = \eta_0 \cdot exp[B/(T - T_0)] \quad (3)$$

$$\kappa = \kappa_0 \cdot exp[-B/(T - T_0)] \quad (4)$$

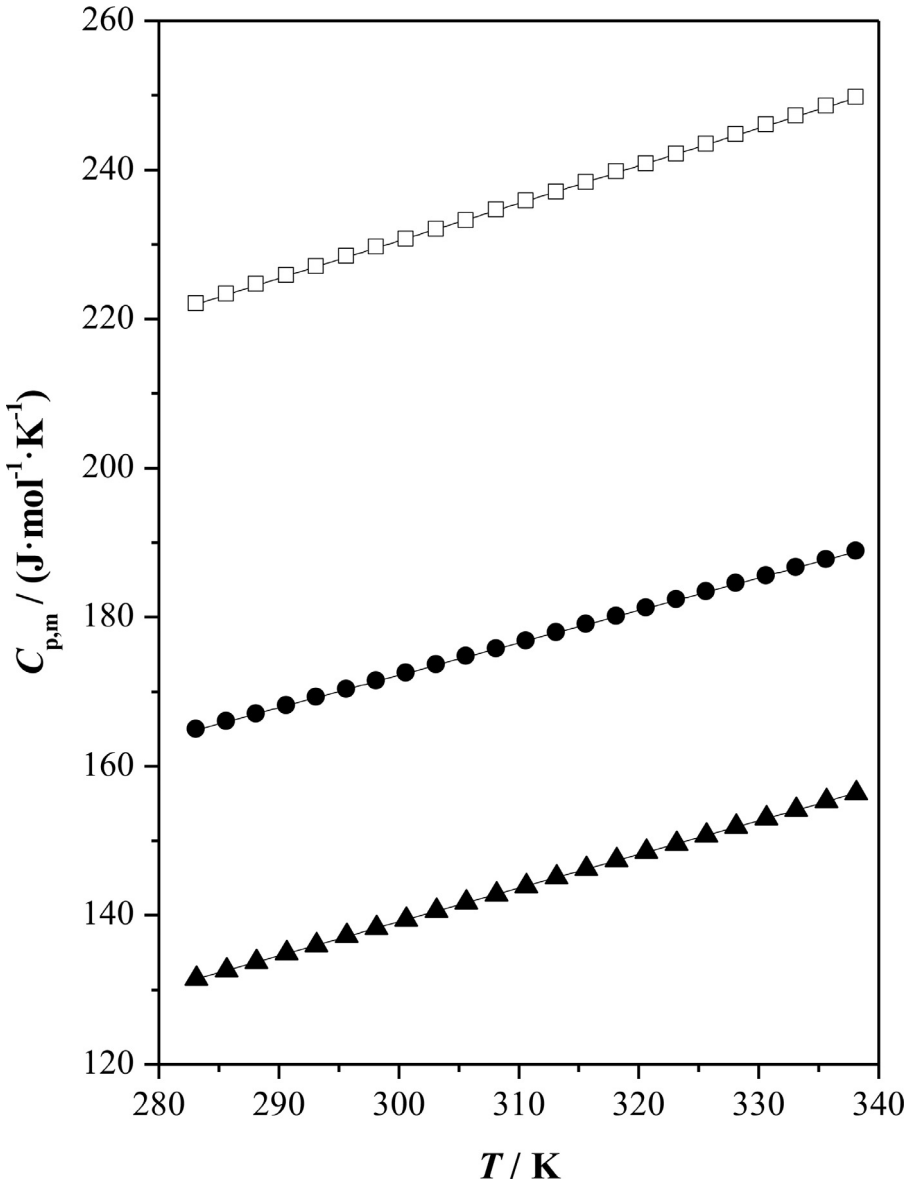

Fig. 8. Isobaric molar heat capacity, $C_{p,m}$, as a function of temperature, T, at $p = 0.1$ MPa for the studied systems: choline chloride:resorcinol (1:2) (□); choline chloride:resorcinol:water (1:2:1.05) (●); choline chloride:resorcinol:water (1:2:2.22) (▲); (—) correlated values.

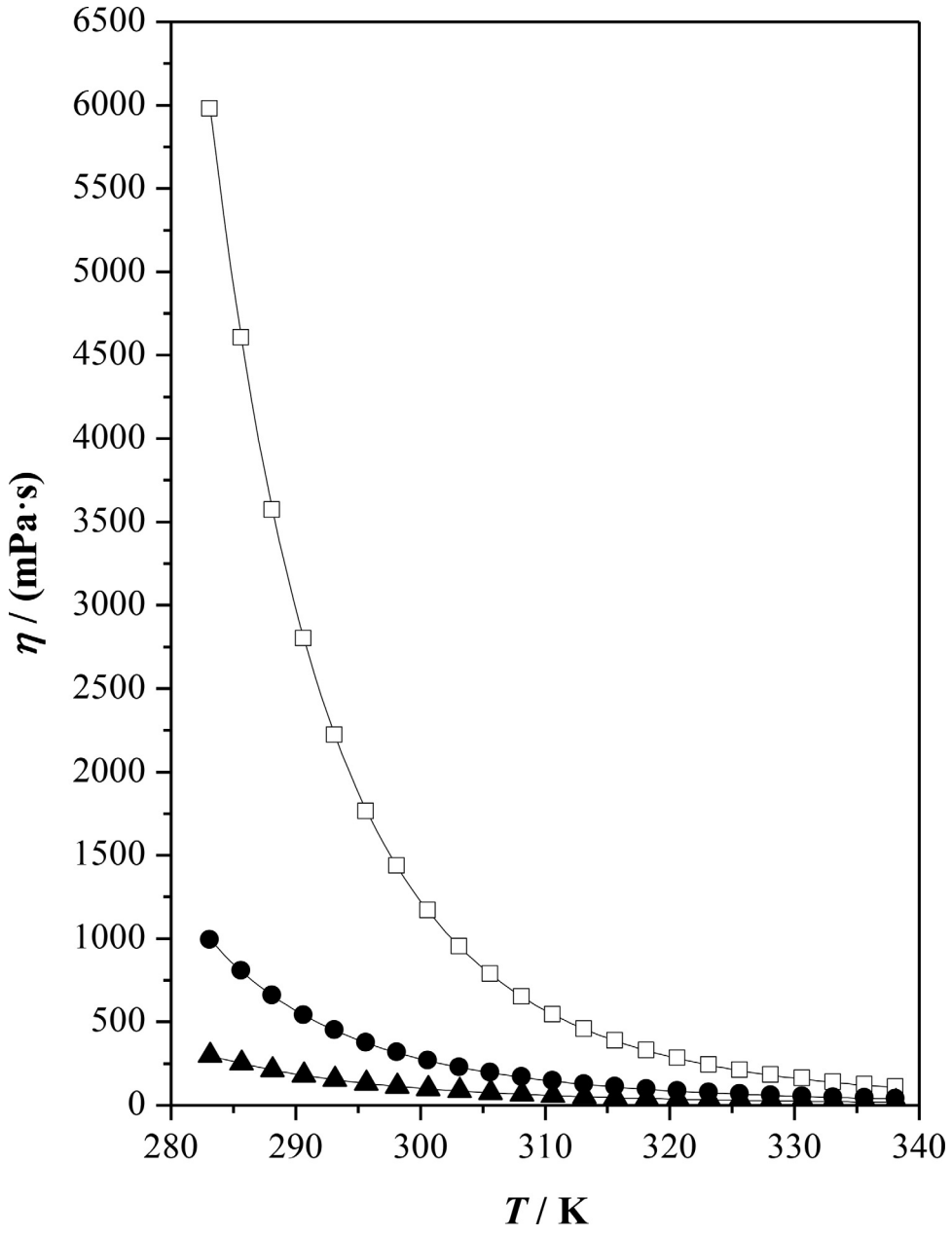

Fig. 9. Dynamic viscosity, η, as a function of temperature, T, at $p = 0.1$ MPa for the studied systems: choline chloride:resorcinol (1:2) (□); choline chloride:resorcinol:water (1:2:1.05) (●); choline chloride:resorcinol:water (1:2:2.22) (▲); (—) correlated values.

where η_0 or κ_0, B and $T_{0\ are}$ the fitting parameters. These parameters along with the corresponding relative root-mean square deviations are also included in Table 2.

Values for the dynamic viscosity vary in the range of 100–1000 mPa·s and depend on the nature of its components, mole ratio, temperature and water content [32]. For our systems at $T = 298.15$ K, the obtained values are 1435 mPa·s, 314.7 mPa·s and 113.1 mPa·s for ChCl:resorcinol (1:2), ChCl:resorcinol:water (1:2:1.05) and ChCl:resorcinol:water (1:2:2.22), respectively. The mixture without water presents higher dynamic viscosity values, which makes it less applicable in industrial processes. On the other hand, mixtures with water present viscosity values of 4.6 and 12.7 times lower than the pure DES. These very marked differences between DES with and without water can be produced due to the intermolecular interactions between resorcinol and water. In all cases, dynamic viscosity decreases exponentially with temperature [41].

Electrical conductivity values are small ($\kappa < 2$ mS·m^{-1}) because of the higher viscosity data. Viscosity decreases with temperature, while electrical conductivity increases [42]. Temperature will increase the velocity of molecules in the liquid and decrease the internal resistance of the molecules. Additionally, the hydrogen bonds formed between HBA and HBD will be weaker when the temperature increases, which means that the viscosity will be lower [41,43].

Electrical conductivity presents higher values for mixtures with water than pure ChCl:resorcinol. This property at $T = 338.15$ K is three times higher for ChCl:resorcinol:water (1:2:1.05) and six times higher for ChCl:resorcinol:water (1:2:2.22) than ChCl:resorcinol (1:2). Viscosity and electrical conductivity are completely related for liquids; in general, chemicals with lower viscosity values present larger conductivity values. In this case, ChCl:resorcinol:water (1:2:2.22) is the compound that presents lower values of viscosity and therefore higher values of electrical

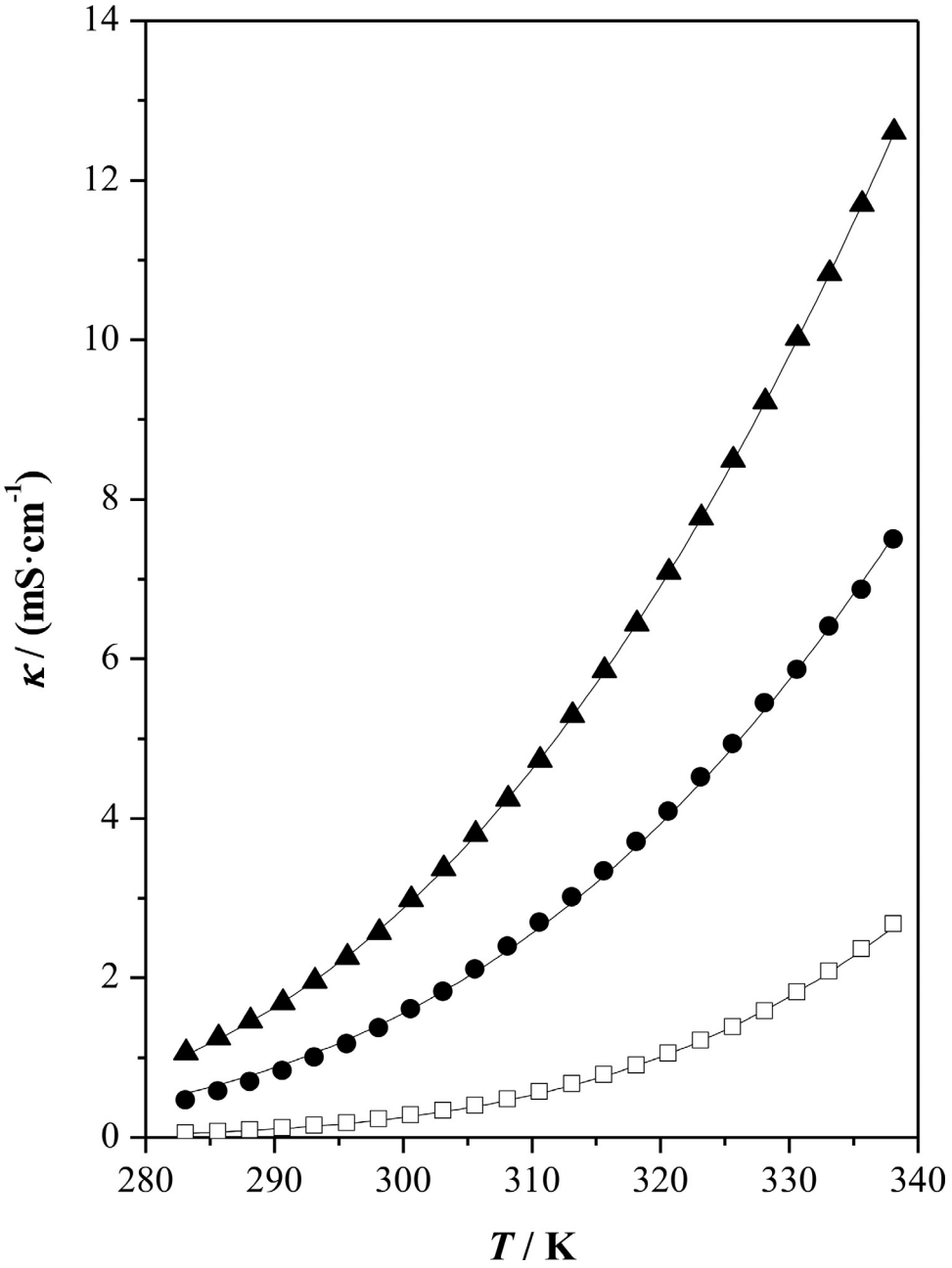

Fig. 10. Electrical conductivity, κ, as a function of temperature, T, at p = 0.1 MPa for the studied systems: choline chloride:resorcinol (1:2) (□); choline chloride:resorcinol:water (1:2:1.05) (●); choline chloride:resorcinol:water (1:2:2.22) (▲); (—) correlated values.

conductivity. For all studied mixtures, this property increases exponentially as temperature increases.

4. Conclusions

In this work, the preparation and a complete physicochemical characterization of ChCl:resorcinol (1:2) and its mixtures with water (ChCl:resorcinol:water (1:2:1.05) and ChCl:resorcinol:water (1:2:2.22)) have been conducted. From the structural characterization (NMR), it was observed that the most intense peaks were found between the hydroxyls of resorcinol and the methyl ones of choline. In the case of thermophysical studies, the properties (density, refractive index, surface tension, isobaric molar heat capacity, viscosity and electrical conductivity) were measured in the following range of temperature T = 283.15 K to 338.15 K) at 0.1 MPa of pressure. The speeds of sound were obtained from T = 308.15 K to 338.15 K. From experimental data, related properties such as isentropic compressibility have been obtained. The results show that a linear correlation with temperature was obtained for most properties (density, speed of sound, refractive index, surface tension, and isobaric molar heat capacity). The viscosity and electrical conductivities can be adjusted using the Vogel-Fulcher-Tammann equation. Finally, the inclusion of water was analysed, from which we observed modifications in all properties, especially in the case of viscosity and electrical conductivity. The inclusion of water leads to a variation in properties. Experimental values decreased as the amount of water increased, with the diminishment of viscosity being the greatest observed effect; this trend can be seen in all the studied properties except for isentropic compressibility, surface tension or electrical conductivity.

Table 2
Fitting parameters, *A*, *B*, and *C*, for the correlation equations and their corresponding root-mean square relative deviations, $RMSD_r$.

Property	Equation	*A*	*B*	*C*	$RMSD_r$/%
Choline chloride:resorcinol (1:2)					
ρ/(kg·m^{-3})	1	−0.5339	1343.37		0.00
u/(m·s^{-1})	1	−2.1380	2531.31		0.04
n_D	1	$-2.38\cdot10^{-4}$	1.6198		0.00
σ/(mN·m^{-1})	1	−0.0441	74.51		0.02
$C_{p,m}$/(J·mol^{-1}·K^{-1})	1	0.504	79.3		0.03
η/(mPa·s)	2	0.0182	1501.4	164.98	0.51
κ/(mS·cm^{-1})	3	3438.4	1119.29	182.18	0.99
Choline chloride:resorcinol:water (1:2:1.05)					
ρ/(kg·m^{-3})	1	−0.5327	1334.26		0.00
u/(m·s^{-1})	1	−2.0392	2482.08		0.03
n_D	1	$-2.47\cdot10^{-4}$	1.6112		0.00
σ/(mN·m^{-1})	1	−0.0417	74.37		0.02
$C_{p,m}$/(J·mol^{-1}·K^{-1})	1	0.435	41.7		0.02
η/(mPa·s)	2	0.0299	1260.5	162.07	0.49
κ/(mS·cm^{-1})	3	397.0	532.84	204.13	0.63
Choline chloride:resorcinol:water (1:2:2.22)					
ρ/(kg·m^{-3})	1	−0.5398	1328.59		0.00
u/(m·s^{-1})	1	−1.9532	2444.06		0.03
n_D	1	$-2.47\cdot10^{-4}$	1.6006		0.00
σ/(mN·m^{-1})	1	−0.0409	74.69		0.02
$C_{p,m}$/(J·mol^{-1}·K^{-1})	1	0.453	3.2		0.03
η/(mPa·s)	2	0.0514	1027.9	164.6	0.45
κ/(mS·cm^{-1})	3	1105.1	686.8	184.64	0.67

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Laura Lomba: Writing – original draft, Supervision. **Federica Tucciarone:** Investigation. **Beatriz Giner:** Formal analysis, Validation. **Manuela Artal:** Writing – original draft. **Carlos Lafuente:** Investigation, Validation, Supervision.

Acknowledgments

The PLATON research group acknowledges financial support from the Gobierno de Aragón and the Fondo Social Europeo “Construyendo Europa desde Aragón” E31_20R. Furthermore, we want to thank Ignacio Delso (Departamento de Síntesis y Estructura de Biomoléculas, Instituto de Síntesis Química y Catálisis Homogénea (ISQH), Universidad de Zaragoza-CSIC) for his contribution to the NMR characterization.

Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.fluid.2022.113435.

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