Experimental and theoretical study on physical properties of the systems dimethyl carbonate and diethyl carbonate + pentanol isomers

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ABSTRACT

In many industrial applications that involve solvents, the knowledge of both thermodynamics properties and transport properties play an important role in the design, sustainability, and optimization of processes in different fields of study. However, it is a fact that there is a lack of data and predictive models for the develop of future applications.

Taking this into account, in this work we studied the physical properties of carbonates and pentanol isomers as well as their mixtures due to the versality of these solvents in many processes. We present measurements of densities (ρ) and excess molar volumes and enthalpies (V_m^E, H_m^E) at 298.15 K for the systems dimethyl or diethyl carbonate + pentanol isomers; and specifically for the systems with diethyl carbonate the surface tensions (σ) and the surface tension deviations ($\delta\sigma$) at 298.15 K and the viscosities (η), dynamic viscosity deviations ($\Delta\eta$), refractive indexes (n_D) and the changes in the refractive index (Δn_D) at 298.15 and 308.15 K. Different theoretical models were applied to obtained data for surface tensions and refractive indexes.

1. Introduction

Nowadays, the ecological transition and change of economic paradigm towards a sustainable consumption boost the development of actions that reduce our environmental impact. This implies an energy and industrial transition where the key point is the development of efficient, sustainable, and environmentally friendly processes.

The concept of sustainable development gives rise to the search for a "green chemistry" in which solvents play an important role. Chemical, chemical engineering and biological processes require the use of solvents that in their majority are or become to be hazardous substances with an important environmental impact. In this regard, different strategies are being adopted to minimize their impact, from the design of solvent-free processes to looking for alternatives to recover, reuse and recycle solvents as well as to substitute traditional solvents for less pollutant alternatives [1–3].

The replacement of the current solvents implies both the discovery of new materials or substances and the modification of existing ones by means of their mixtures with other solvents or additives. Considering that the number of solvents available is enormous, the resulting mixture should have at least similar or better properties than the original solvent and, in turn, be environmentally friendly. It becomes necessary to have an experimental database of physicochemical properties both of pure components and their mixtures to help us not only in the selection of solvents but also in the development of theoretical models that explain and predict the behaviour of their mixtures.

In this context, we have selected for their study a pair of carbonates dimethyl carbonate (DMC) and diethyl carbonate (DEC) and a series of alcohols such as the 1-pentanol (1-ol) and their isomers 2-pentanol (2-ol), 3-pentanol (3-ol), 2-methyl-1-butanol (2,1-ol), 2-methyl-2-butanol (2,2-ol), 3-methyl-1-butanol (3,1-ol) and 3-methyl-2-butanol (3,2-ol).

DMC and DEC are one of the organic solvents most widely used not only because of its high oxygen content but also for being considered as replacements for other substances more harmful to the environment such as methyl-*tert*-butyl ether in fuels or methyl halides and phosgene in reactions of methylation and carbonylation. They can also be used as solvents in paints and adhesives as well as chemical intermediates in reactions of polycarbonates, polyurethanes, drugs, or as electrolytes in batteries. In fact, both DMC and DEC are the organic solvents commonly used in lithium batteries. Currently, there is no doubt about the

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Table 1

Chemical name, molar mass, provenance, mass fraction purity, CAS number, and chemical structures of the compounds studied in this work.

Chemical name	M/g•mol^{-1}	Provenance	Purity	CAS number	Chemical structure
Dimethyl carbonate (DMC)	90.08	Sigma-Aldrich	0.99	616-38-6	
Diethyl carbonate (DEC)	118.13	Aldrich	0.99	105-58-8	
1-pentanol (1-ol)	88.15	Fluka	≥0.99	71-41-0	
2-pentanol (2-ol)	88.15	Aldrich	0.98	6032-29-7	
3-pentanol (3-ol)	88.15	Aldrich	0.98	584-02-1	
2-methyl-1-butanol (2,1-ol)	88.15	Aldrich	≥0.99	137-32-6	
2-methyl-2-butanol (2,2-ol)	88.15	Sigma-Aldrich	≥0.99	75-85-4	
3-methyl-1-butanol (3,1-ol)	88.15	Sigma-Aldrich	≥0.99	123-51-3	
3-methyl-2-butanol (3,2-ol)	88.15	Aldrich	0.98	598-75-4	

importance of the development of this kind of batteries because of the use of handheld devices such as laptops, mobiles phones, … However, although the carbonates are characterised by their stability with lithium salts, these present several problems of safety due to their flammability and volatility. For these reasons, many of the research efforts in this field are directed at finding new electrolytes or improving the existing ones with the inclusion of additives [4–18].

On the other hand, alcohols such as pentanol and its isomers are used in the production of biofuels and as an additive in gasoline blends, lubrication oil, plastics… as well as solvents or chemical intermediates in processes of production for paints, coatings, pharmaceutical products, cosmetics… [19–27].

The versatility and applicability of these substances as well as the lack of experimental data in the literature make the study of the physicochemical properties of their mixtures necessary. Properties such as density, viscosity, and surface tension are particularly important because they help us to understand the nature of the fluids under different conditions of temperature, pressure, etc. In this way, we can select the appropriate fluid for a given application and relate it to the manufacturing processes with a view to optimizing and innovating successful future designs.

In this work, we present the densities (ρ), excess molar volumes and enthalpies (V_m^E, H_m^E) at 298.15 K for the systems dimethyl or diethyl carbonate + pentanol isomers; the surface tensions (σ) and the surface tension deviations (δσ) for the systems diethyl carbonate + pentanol isomers at 298.15 K and viscosities (η), dynamic viscosity deviations (Δη), refractive indexes (n_D) and their changes in the refractive index (Δn_D) at 298.15 and 308.15 K for the systems diethyl carbonate + pentanol isomers.

In the literature, there is a lack of published data on surface tensions for all studied systems at 298.15 K. Also, we could not find data either for ρ, η, V_m^E, and n_D for all mixtures of DEC + pentanol isomers at 298.15 K -except for those containing 1-pentanol- or for data on η and n_D at 308.15 K [28–31]. All values at atmospheric pressure.

In the case of the systems of DMC + pentanol isomers data of ρ and

H_m^E at 298.15 K were missing while we did find density data on the binary systems DMC + 1-ol and DMC + 2-ol [32,33].

2. Experimental section

2.1. Chemicals

The compounds studied are shown in Table 1, where we indicate the chemical name, the acronyms, the molecular weight, as well as their provenance, mass fraction purity, CAS number, and chemical structure. The compounds were used as they came from the dealer without any additional purification in our laboratory. At the same time, these were degassed by ultrasounds and dried in over 0.4 nm molecular sieve before being used.

2.2. Apparatus and procedure

All binary mixtures were weighed using a Mettler AT 201 balance with a relative standard uncertainty of $1 \cdot 10^{-4}$.

As a first step, we measured the density (ρ), and excess molar enthalpy (H_m^E) of the binary systems DMC or DEC + pentanol isomers (1-ol, 2-ol, 3-ol, 2,1-ol, 2,2-ol, 3,1-ol and 3,2-ol) at 298.15 K. The measurements of viscosity (η) and refractive index (n_D) of the binary systems DEC + pentanol isomers were performed at 298.15 and 308.15 K, whereas the surface tension was measured at 298.15 K. All measurements have been performed at atmospheric pressure about 101 kPa.

The experimental measurements of the excess molar enthalpies (H_m^E) were carried out using a Calvet heat flow microcalorimeter. The calibration and the operating conditions were described by Verdes et al. [34]. This microcalorimeter works with a calorimeter cell whose volume is about 10 cm^3 and is equipped with a device allowing operation in the absence of the vapour phase. It is connected to Philips PM2535 multimeter and a data acquisition system. The microcalorimeter was calibrated electrically using a stabilized current source EJP 30 Setaram and subsequently it was checked by determining excess enthalpies for the standard system (n-hexane + cyclohexane) at 298.15 K. The uncertainty

Table 2

Physical properties of the compounds used in this work with results available in the literature at 101 kPa[a].

Compound	ρ/g·cm^{-3}		η/mPa·s				σ/mN·m^{-1}		n_D			
	Exp.	Lit.	Exp.	Lit.	Exp.	Lit.	Exp.	Lit.	Exp.	Lit.	Exp.	Lit.
	T = 298.15 K		T = 298.15 K		T = 308.15 K		T = 298.15 K		T = 298.15 K		T = 308.15 K	
DEC	0.96910	0.96906 [38] 0.96912 [39]	0.7802	0.764 [40] 0.757 [41,42]	0.6885	0.664 [42] 0.659 [43]	25.62	25.43 [44] 25.87 [45]	1.38225	1.38240 [46] 1.38252 [47]	1.37756	1.37769 [47] 1.3780 [48]
DMC	1.06310	1.06310 [49,50] 1.06311 [51]										
1-Pentanol	0.81101	0.8110 [52] 0.81100 [53]	3.502	3.501 [54] 3.505 [53]	2.659	2.650 [53] 2.648 [55]	24.95	24.97 [56] 24.89 [57]	1.40797	1.4082 [52] 1.40798 [58]	1.40392	1.40379 [59] 1.40388 [60]
2-Pentanol	0.80480	0.8047 [61] 0.80497 [62]	3.386	3.381 [61] 3.46 [63]	2.330	2.340 [64] 2.35 [63]	23.34	23.30 [65] 23.28 [66]	1.40442	1.4044 [63] 1.4042 [52]	1.39991	1.4002 [63] 1.40029 [67]
3-Pentanol	0.81548	0.8155 [63,52]	4.543	4.69 [63]	2.787	2.7726 [68] 2.82 [63]	23.98	24.60[b] [69] 23.76[c] [69]	1.40836	1.4081 [63] 1.40826 [70]	1.40333	1.4037 [63] 1.4029 [71]
2-Methyl-1-butanol	0.81504	0.81502 [72] 0.81511 [53]	4.505	4.501 [54] 4.512 [53]	3.188	3.258 [64] 3.265 [54]	24.20	24.03 [65]	1.40861	1.40866 [73] 1.4086 [72]	1.40434	1.40447 [74]
2-Methyl-2-butanol	0.80426	0.804257 [75] 0.80428 [76]	3.463	3.4781 [77] 3.533 [78]	2.325	2.2151 [79] 2.72 [80]	22.51	22.77[b] [79] 21.89[c] [79]	1.40261	1.4025 [81] 1.4029 [82]	1.39749	1.3968 [77]
3-Methyl-1-butanol	0.80459	0.8046 [80] 0.80439 [83]	3.681	3.63 [80] 3.671 [84]	2.745	2.72 [80] 2.730 [84]	23.02	23.71 [85]	1.40465	1.40469 [84] 1.40451 [83]	1.40046	1.40051 [84] 1.4008 [86]
3-Methyl-2-butanol	0.81303	0.8128 [69] 0.81375 [82]	4.159	3.161[c] [87] 3.163[c] [69]	2.652	3.161[c] [87] 3.163[c] [69]	23.07	23.0 [69]	1.40739	1.4074 [88] 1.4075 [69,82]	1.40247	–

[a] Standard uncertainty: u(T) = 0.02 K, u(P) = 1 kPa, u(ρ) = 0.02 kg•m^{-3}, u(σ) = 0.02 mN·m^{-1}. Combined expanded uncertainty: U(n_D) = 0.0005. Relative combined expanded uncertainty u$_r$(η) = 0.01.
[b] T = 293.15 K.
[c] T = 303.15 K.

of the excess molar enthalpies is estimated as better than 1 %.

Density (ρ) was measured with an Anton Paar DMA 60/602 vibrating tube densimeter with a standard uncertainty about 0.02 kg·m^{-3}. A Schott-Geräte CT 1450 circulating water bath was regulated to maintain the cell temperature with a standard uncertainty of 0.02 K that was taken with an Anton Paar DT 100-20 digital thermometer. The calibration was made with Milli-Q water and with heptane (Sigma > 0.99).

Dynamic viscosity (η) measurements were carried out in an Anton Paar SVM 3000 Stabinger viscodensimeter, which was thermostated with an internal Peltier cell with an uncertainty of 0.02 K. The procedure of measurement was detailed previously [35]. The relative combined expanded uncertainty of viscosity is 0.01 of the measured value. Also, the viscosity value range goes from 0.2 up to 20,000 mPa·s, which is enough to measure these substances in a wide temperature range. This equipment is checked with reference chemicals recommended by the supplier M114 and C117 SH Calibration Service GmbH.

Surface tension (σ) was determined using a Lauda TVT1 automated tensiometer, which employs the principle of the drop volume. The technique consists of measuring the volume of a drop detaching from a capillary with a circular cross section. Detailed instrument design and experimental procedure have been described elsewhere [36]. The standard uncertainty of the measurement is 0.02 mN·m^{-1}. A Lauda RC6 CP thermostatic bath controlled the temperature to better than 0.2 K. We need to know the density of the mixtures to calculate the surface tension from the drop volume measured by the tensiometer. This density was measured with an Anton Paar SVM 3000 Stabinger viscodensimeter. The

combined expanded uncertainty in the measurement with a coverage factor, k, of 2 of density is about 0.5 kg·m^{-3}. This viscodensimeter automatically corrects the density value depending on the viscosity of the sample.

Refractive index (n_D) was measured in an Anton Paar Abbemat Automative refractometer which was thermostated with an internal Peltier cell with an accuracy of ±0.03 K. Details of the refractive index measurement were published previously [37]. The combined expanded uncertainty of the measurements of refractive indexes is 0.0005. The reference fluids used to calibrate were Milli-Q water and cyclohexane (Fluka > 0.995).

Before describing the behaviour of the studied systems, we will a give a summary of the data processing. It is worth noting that unlike the direct measurements of ρ, η, σ, n_D and H_m^E; V_m^E, $\Delta\eta$, $\delta\sigma$ and Δn_D were calculated through the following equations.

$$V_m^E = x_1 M_1 \left(\frac{1}{\rho} - \frac{1}{\rho_1} \right) + x_2 M_2 \left(\frac{1}{\rho} - \frac{1}{\rho_2} \right) \tag{1}$$

$$\Delta\eta = \eta - x_1\eta_1 - x_2\eta_2 \tag{2}$$

$$\delta\sigma = \sigma - x_1\sigma_1 - x_2\sigma_2 \tag{3}$$

$$\Delta n_D = n_D - x_1 n_{D1} - x_2 n_{D2} \tag{4}$$

where ρ, η, σ and n_D are the density, viscosity, the surface tension, and the refractive index in the mixture; x_1 and x_2 are the molar fraction
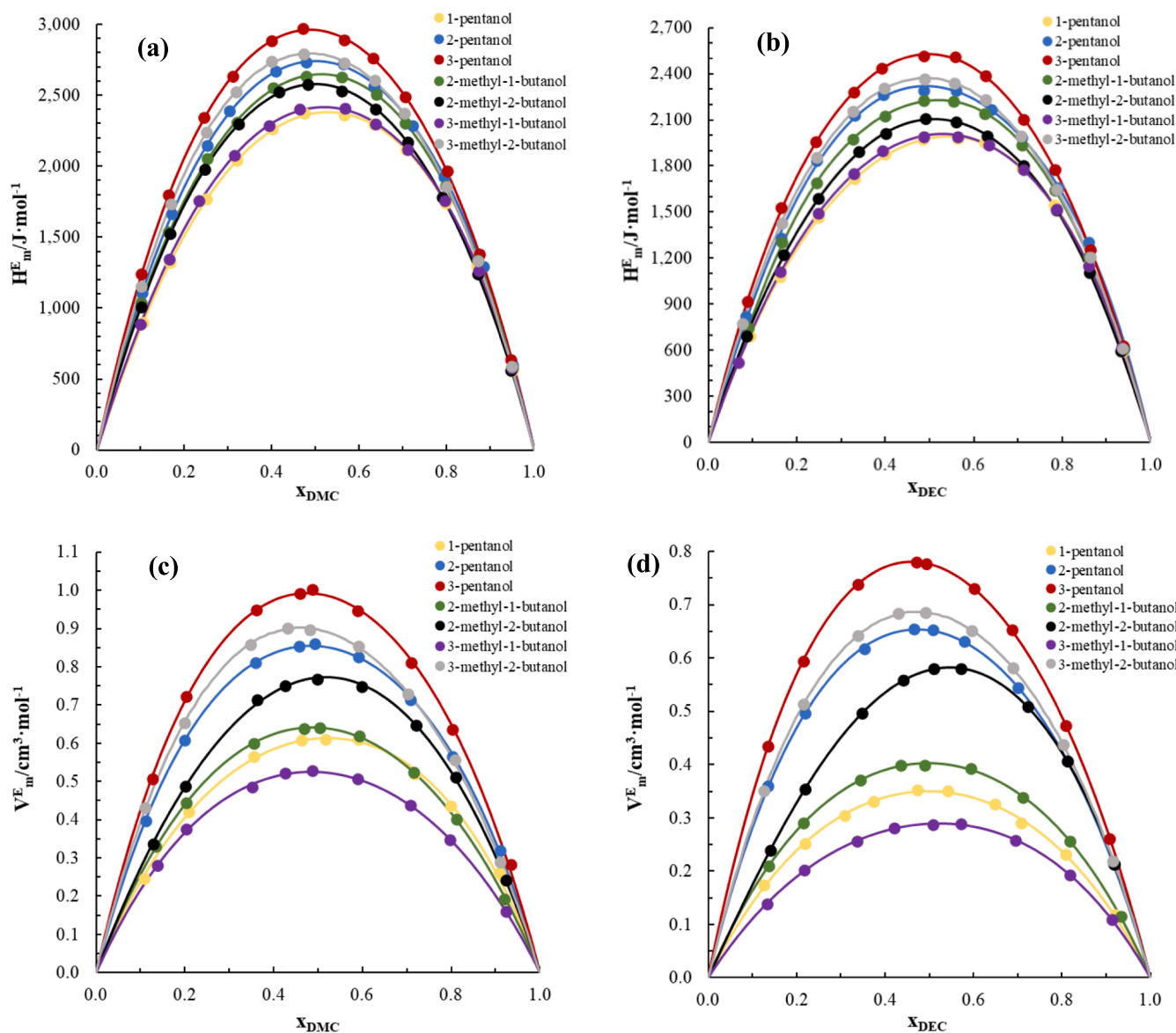
Fig. 1. Excess molar enthalpies and volumes of (a), (c) DMC + pentanol isomers and (b), (d) DEC + pentanol isomers at 298.15 K. The continuous lines correspond to the fit of a Redlich-Kister equation (Eq. (5)).

of the component 1 (DMC or DEC) and component 2 (pentanol isomers) and ρ_1, ρ_2, η_1, η_2, σ_1, σ_2, n_{D1} and n_{D2} are the properties of the corresponding pure components.

3. Results and discussion

All measurements were carried out at atmospheric pressure of 101 kPa and standard uncertainty 1 kPa. The experimental values of the compounds used and their comparison with those previously published are given in Table 2. The experimental data show a percentage relative deviations between 0.001 %–0.09 % for densities, 0.03 %–3 % for viscosities, 0.08 %–3 %, and 0.0007 %–0.02 % for surface tensions and refractive indexes, respectively. At 308.15 K the intervals of the percentage relative deviation are from 0.3 % to 5 % for viscosities and from 0.004 % to 0.05 % for the case of refractive indexes.

Fig. 1 (a) and (b) show the excess molar enthalpies (Table S1) and (c) and (d) excess molar volumes (Table S2) of binary systems DMC or DEC + pentanol isomers at 298.15 K. The data of H^E_m and V^E_m for all the studied mixtures were fitted to equation (5) proposed by Redlich-Kister

whose fit parameters are given in Table 3.

Both magnitudes are positive in the whole concentration range as the result of the reorganization of intermolecular forces that occur in the mixing process as well as the differences between the size and form of their components. If we analyse the individual components of the mixtures, carbonate molecules DMC or DEC interact with each other through dipole–dipole interactions whereas isomers of pentanol molecules are attracted by hydrogen bonds between their hydroxyl groups. When these two components are mixed the hydrogen bonds of the isomers of pentanol are broken and dipole–dipole interactions between alcohols and carbonates are formed [51,89]. The resulting energy balance between the formation and rupture of the interactions that take place in this process leads to positive values for both H^E_m and V^E_m which in turn are influenced by the structural characteristics of the components of the mixture.

The maximum values of the H^E_m of mixtures carbonate + alkanol are all near to 0.5 M fraction of carbonate and vary between 2970 and 2371 J·mol^{-1} for the case of DMC mixtures and 2500 and 1970 J·mol^{-1} for the mixtures with DEC whereas in the case of the V^E_m, the maximum values

Table 3

Coefficients A_k from equation (5) and standard deviations, s.

	A_0	A_1	A_2	A_3	A_4	A_5	s
DMC + 1-pentanol (T = 298.15 K)							
H_m^E (J·mol^{-1})	9511	875.1	1742	681.8			5
V_m^E (cm^3·mol^{-1})	2.449	0.1715	0.5276				0.0092
DMC + 2-pentanol (T = 298.15 K)							
H_m^E (J·mol^{-1})	10,967	−32.83	2080	602.5			7
V_m^E (cm^3·mol^{-1})	3.417	−0.1729	0.7986				0.0049
DMC + 3-pentanol (T = 298.15 K)							
H_m^E (J·mol^{-1})	11,842	−512.4	2046				7
V_m^E (cm^3·mol^{-1})	3.961	−0.3194	0.7948				0.0094
DMC + 2-methyl-1-butanol (T = 298.15 K)							
H_m^E (J·mol^{-1})	10,587	438.8	1866				8
V_m^E (cm^3·mol^{-1})	2.564	−0.1169	0.3146				0.0021
DMC + 2-methyl-2-butanol (T = 298.15 K)							
H_m^E (J·mol^{-1})	10,312	−32.85	1318				7
V_m^E (cm^3·mol^{-1})	3.086	0.2035	0.1877				0.0048
DMC + 3-methyl-1-butanol (T = 298.15 K)							
H_m^E (J·mol^{-1})	9658	600.9	1790	799.5			8
V_m^E (cm^3·mol^{-1})	2.101	−0.1101	0.3483				0.0034
DMC + 3-methyl-2-butanol (T = 298.15 K)							
H_m^E (J·mol^{-1})	11,174	−481.6	2395	182.0	−995.5		6
V_m^E (cm^3·mol^{-1})	3.588	−0.4791	0.6441				0.0043
DEC + 1-pentanol (T = 298.15 K)							
H_m^E (J·mol^{-1})	7930	1078	1669				6
V_m^E (cm^3·mol^{-1})	1.402	−0.0095	0.2433				0.0035
$\Delta\eta$ (mPa·s)	−4.004	2.298	−2.160	1.967	−0.389		0.0087
$\delta\sigma$ (mN·m^{-1})	−0.6778	0.0707	0.7253	1.1335	0.5273		0.0018
Δn_D	−0.0076	0.0013	0.0003	−0.0004			0.00014
DEC + 2-pentanol (T = 298.15 K)							
H_m^E (J·mol^{-1})	9277	−277.4	2050	1302			20
V_m^E (cm^3·mol^{-1})	2.610	−0.2301	0.5173				0.0020
$\Delta\eta$ (mPa·s)	−4.393	3.241	−1.960	0.739	−1.933	2.266	0.0044
$\delta\sigma$ (mN·m^{-1})	−0.5561	0.1185	1.0708	0.2948			0.014
Δn_D	−0.0108	0.0025	−0.0022	0.0005			0.00007
DEC + 3-pentanol (T = 298.15 K)							
H_m^E (J·mol^{-1})	10,119	−86.59	1482	−489.3			8
V_m^E (cm^3·mol^{-1})	3.105	−0.4157	0.5710				0.0018
$\Delta\eta$ (mPa·s)	−6.660	5.305	−4.323	2.672	−3.366	4.113	0.0014
$\delta\sigma$ (mN·m^{-1})	−1.1445	−0.1703	−0.1636				0.0074
Δn_D	−0.0128	0.0016	−0.0008	0.0025			0.00003
DEC + 2-methyl-1-butanol (T = 298.15 K)							
H_m^E (J·mol^{-1})	8896	554.3	2213	−1080	−1533	1974	5
V_m^E (cm^3·mol^{-1})	1.609	−0.0143	0.2981				0.0015
$\Delta\eta$ (mPa·s)	−6.126	4.222	−3.222	2.952	−1.205		0.013
$\delta\sigma$ (mN·m^{-1})	−0.6151	0.0272	−0.0156				0.0039
Δn_D	−0.0087	−0.0005	0.0033				0.00018
DEC + 2-methyl-2-butanol (T = 298.15 K)							
H_m^E (J·mol^{-1})	8416	289.0	1165	808.4	−219.4	−1099	3
V_m^E (cm^3·mol^{-1})	2.311	0.4132	0.1057	0.2219			0.0006
$\Delta\eta$ (mPa·s)	−4.384	3.075	−2.433	1.976	−0.878		0.0083
$\delta\sigma$ (mN·m^{-1})	−1.6501	−0.0753	−0.5919				0.0063
Δn_D	−0.0098	−0.0010	−0.0030	−0.0001			0.00002
DEC + 3-methyl-1-butanol (T = 298.15 K)							
H_m^E (J·mol^{-1})	8004	754.2	1615	402.5			5
V_m^E (cm^3·mol^{-1})	1.156	0.0823	0.2154				0.0015
$\Delta\eta$ (mPa·s)	−4.532	2.692	−1.561	2.342	−1.377	−1.016	0.0018
$\delta\sigma$ (mN·m^{-1})	−0.3453	−0.0519	0.3993	0.2362			0.0043
Δn_D	−0.0061	−0.0001	−0.0005				0.00003
DEC + 3-methyl-2-butanol (T = 298.15 K)							
H_m^E (J·mol^{-1})	9490	−268.4	1562				4
V_m^E (cm^3·mol^{-1})	2.740	−0.2500	0.4739				0.0020
$\Delta\eta$ (mPa·s)	−5.790	4.329	−2.846	1.812	−3.523	3.594	0.011
$\delta\sigma$ (mN·m^{-1})	−0.8535	0.0159	0.7290	−1.2738	0.5054		0.0066
Δn_D	−0.0127	0.0029	−0.0022	−0.0022	0.0026		0.00004
DEC + 1-pentanol (T = 308.15 K)							
$\Delta\eta$ (mPa·s)	−2.806	1.437	−1.690	1.627			0.012
Δn_D	−0.0084	0.0020	−0.0021	0.0002			0.00016
DEC + 2-pentanol (T = 308.15 K)							
$\Delta\eta$ (mPa·s)	−2.715	1.883	−0.992	0.370	−1.025	1.048	0.0034
Δn_D	−0.0115	0.0019	−0.0030	0.0019			0.00007
DEC + 3-pentanol (T = 308.15 K)							
$\Delta\eta$ (mPa·s)	−3.607	2.668	−2.133	1.101	−1.176	1.934	0.00064
Δn_D	−0.0128	0.0002	−0.0009	0.0025			0.00002
DEC + 2-methyl-1-butanol (T = 308.15 K)							
$\Delta\eta$ (mPa·s)	−4.033	2.483	−1.750	3.082	−0.978	−1.924	0.0095

Table 3 (*continued*)

	A_0	A_1	A_2	A_3	A_4	A_5	s
Δn_D	−0.0093	−0.0016	0.0040				0.00013
DEC + 2-methyl-2-butanol (T = 308.15 K)							
$\Delta \eta$ (mPa·s)	−2.599	1.723	−1.422	0.889	−0.052		0.0077
Δn_D	−0.0107	−0.0006	−0.0004	−0.0019			0.00005
DEC + 3-methyl-1-butanol (T = 308.15 K)							
$\Delta \eta$ (mPa·s)	−3.168	1.777	−0.868	1.395	−0.895	−0.668	0.0025
Δn_D	−0.0068	−0.0005					0.00005
DEC + 3-methyl-2-butanol (T = 308.15 K)							
$\Delta \eta$ (mPa·s)	−3.247	2.180	−1.399	1.066	−1.391	1.221	0.0085
Δn_D	−0.0129	0.0020	−0.0017				0.00006
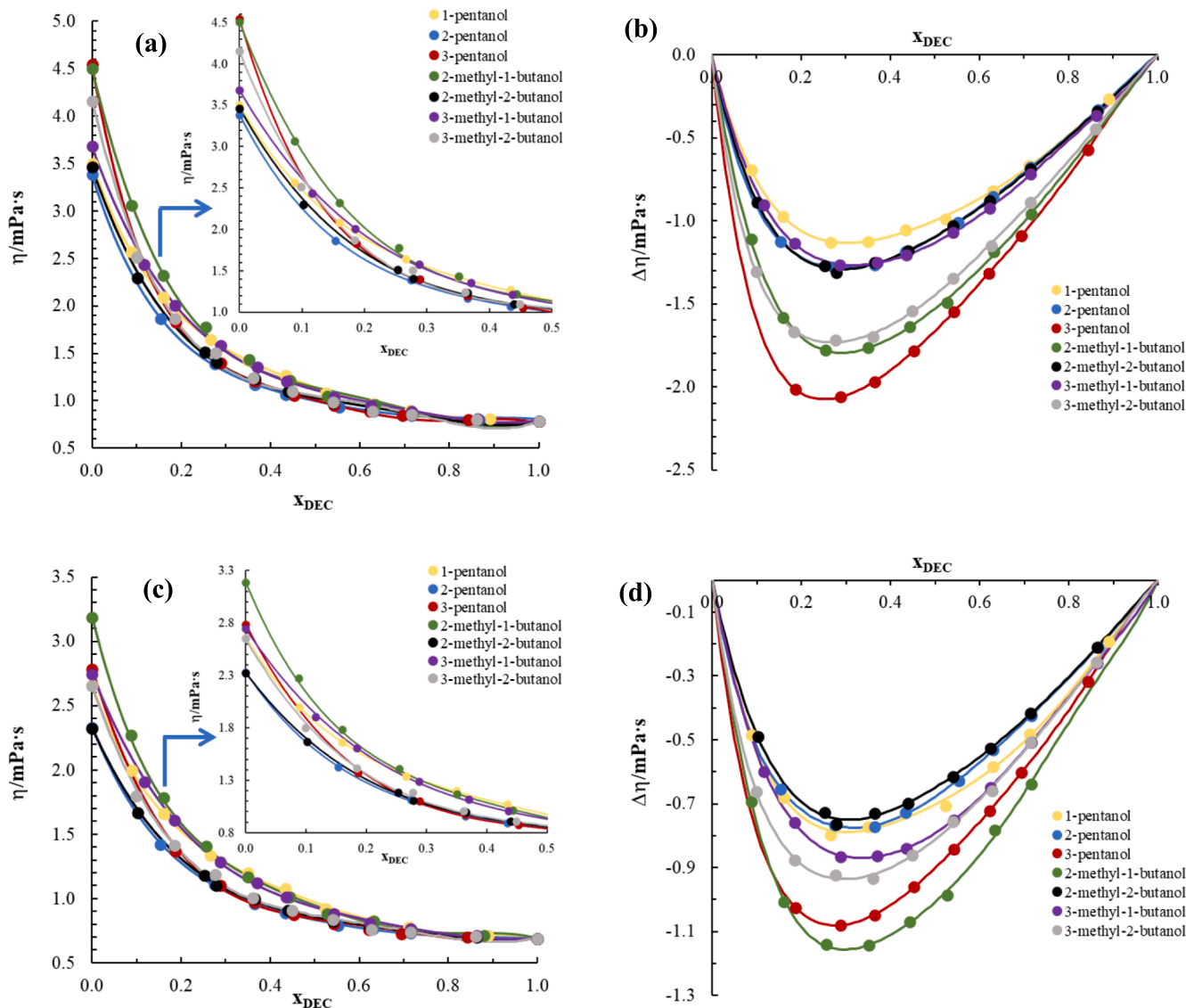
Fig. 2. Viscosities and dynamic viscosity deviations of DEC + pentanol isomers (a) and (b) at 298.15 K and (c) and (d) at 308.15 K. The continuous lines in the viscosities correspond to a polynomial fit. The continuous lines in the dynamic viscosity deviations correspond to the fit of a Redlich-Kister equation (Eq. (5)).

are at mole fractions ≈ 0.5 except for the systems DMC + 3,2-ol, DEC + 2,2-ol and DEC + 3,1-ol which are shifted to $x_{DMC} < 0.5$ and to $x_{DEC} > 0.5$ respectively. These latter show maximum values between 1 and 0.53 cm³·mol⁻¹ for the DMC and between 0.78 and 0.29 cm³·mol⁻¹ for the DEC. The differences obtained between the values of both carbonates can be attributed to the fact that the dipole interactions are larger for the DMC than for the DEC [89].

If we pay attention in the influence of the OH position in the isomers of pentanol on the results, according to whether the OH is on a primary (2,1-ol, 3,1-ol, 1-ol) secondary (3,2-ol, 2-ol, 3-ol) or tertiary carbon (2,2-ol) we observe that the values for H_m^E for the binary systems for both carbonates are as follows 3-ol > 3,2-ol > 2-ol > 2,1-ol > 2,2-ol > 3,1-ol ≈ 1-ol whereas the behaviour of the V_m^E is very similar but with two small differences on the one hand we observe an inversion in the order
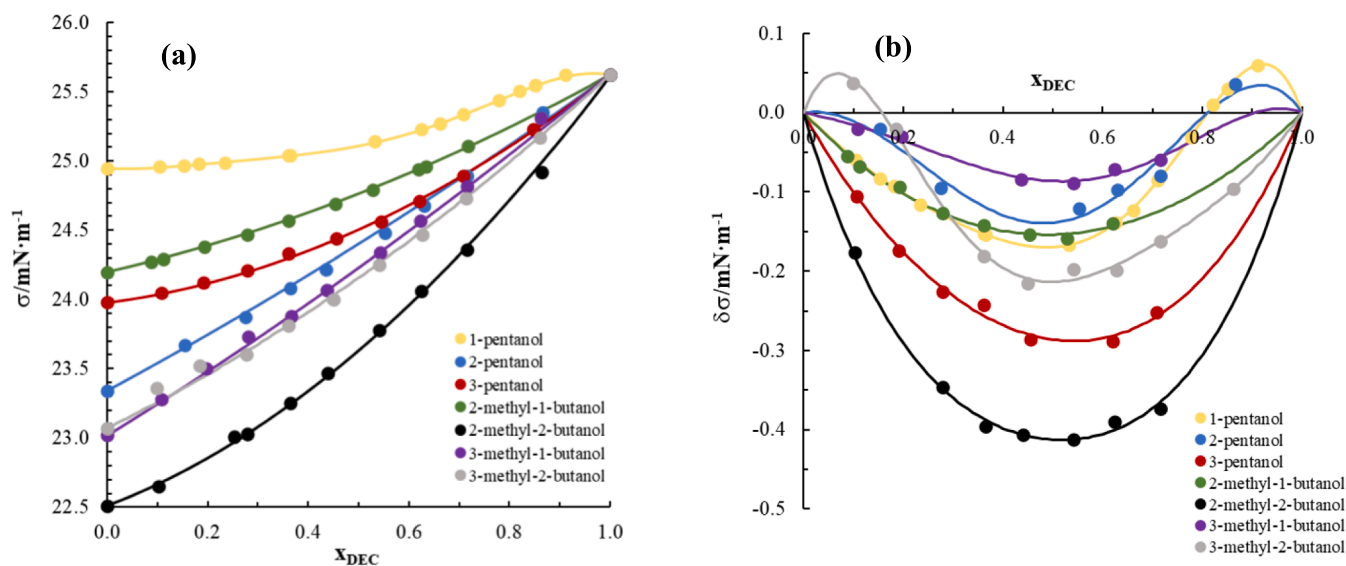
Fig. 3. Surface tensions (a) and surface tension deviations (b) of DEC + pentanol isomers at 298.15 K. The continuous lines in the surface tensions correspond to a polynomial fit. The continuous lines in the surface tension deviations correspond to the fit of a Redlich-Kister equation (Eq. (5)).

between the mixtures of carbonate with 2–1,ol and 2–2,ol and the other hand the values of the mixtures 3,1 ol and 1-ol do not coincide. Likewise, the values of V_m^E are <1 % because of this we can consider the behaviour of these mixtures quasi-ideal.

These values are quite similar between the different isomers, showing the smallest values those pentanol isomers having a hydroxyl group connected to a primary carbon such as 1-pentanol and 3-methyl-1-butanol. As it was explained in previous work [90], the small differences in effective dipole moment, $\bar{\mu}$, of the isomers of pentanol suggest that the influence of dipolar interactions is less important than steric hindrance in the values obtained. Thus, the less branched the alcohol chain is, the better the packing and the smaller the distance between molecules and therefore the lower H_m^E and V_m^E [28,91].

In the literature, no published data was found about H_m^E of the mixtures with DMC while data exist for the systems DEC + pentanol isomers which are in good agreement with those given in the literature [28]. Thus, we found differences of around 1.5 % for systems 1-ol, 2,1-ol, 2,2-ol and 3,1-ol and 5 % for systems 2-ol, 3-ol and 3,2-ol. Regarding V_m^E, we have found a data set for densities and excess molar volumes for DMC or DEC + 1-ol [32,29,31] and DMC + 2-ol [33]. If we compare our data with those published, these show differences of 0.2 % for the densities and 2 % and 45 % for the excess volumes for the systems DMC + 1-ol and DEC + 1-ol respectively.

Moreover, the excess molar volumes and enthalpies, were measured for the mixtures of DEC + pentanol isomers, the surface tension at 298.15 K, the viscosity, and their refractive indexes at the temperatures of 298.15 K and 308.15 K.

The experimental dynamic viscosity data (η) for the compounds studied are shown as a function of the mole fraction of carbonate in Table S3 and illustrated in Fig. 2 (a) and (c) at 298.15 K and 308.15 K. As commonly observed, viscosity values decrease markedly with mole fraction of carbonate increases in a polynomial trend. As regards the dependence of the viscosity with the temperature, the values of the viscosity decrease markedly with temperature increases. Like the excess molar volumes and enthalpies, the viscosities are related to the interaction of the components of the mixture as well as the size and shape of the molecules that make up the mixture. Thus, the calculation of dynamic viscosity deviation ($\Delta\eta$) can give us an idea of the strength of the interactions in the mixing process. Fig. 2 (b) and (d) show the $\Delta\eta$ versus the molar fraction of the carbonate at 298.15 K and 308.15 K. The data were fitted to Redlich-Kister equation whose fit parameters are given in

Table 3. Negative values of the $\Delta\eta$ mean weaker interactions carbonate-alcohol in contrast to the stronger alcohol-alcohol and carbonate-carbonate interactions [92,93]. Positive V_m^E and negative $\Delta\eta$ are indicative of the disruptive effect of the carbonate in the self-associated alcohols leading to an increase in the volume and a decrease of the viscosity [92,94].

The maximum values of $\Delta\eta$ to both temperatures are shifted towards alcohol rich mole fractions $x_{DEC} \approx 0.3$. The distribution of the absolute values of $\Delta\eta$ in relation to the different isomers of pentanol is as follows: 3-ol > 2,1-ol > 3,2-ol > 2,2-ol $\geq$ 2-ol $\geq$ 3,1-ol > 1-ol at 298.15 K and 2,1-ol > 3-ol > 3,2-ol > 3,1-ol > 1-ol > 2-ol > 2,2-ol at 308.15 K. From these results it is worth noting that at the temperature 298.15 K the systems 3,2-ol and 2, 1-ol show similar values as do the systems 2-ol, 2,2-ol and 3,1-ol. However, these values are no longer similar at 308.15 K. In contrast to the enthalpies and volumes, we cannot establish a relationship with the type of the isomer of pentanol.

The values of the system DEC + 1-pentanol at 298.15 K have been previously published [29,30]. The difference between these values and ours is of 2 % for the viscosities and 5 % for $\Delta\eta$.

The surface tension values and their calculated surface tension deviations of DEC + pentanol isomers at 298.15 K are shown in Table S4, Fig. 3 (a) and (b). The surface tension deviations are fitted to Redlich-Kister equation (Eq. (5)) whose parameters are given in Table 3.

The collection of data of surface tension obtained gives us information about the distribution of molecules between the internal volume of liquid, bulk, and the vapor–liquid interface and therefore the tendency of the components to adsorb on the surface of the liquid, that in the case of the mixtures corresponds to the components with the lowest surface tension [95]. It is likely that in the case of our samples, it is the pentanol isomers that are arranged on the surface of the liquid.

In all the systems studied, we observed that the increase of the carbonate mole fraction increases the mixing surface tension. The highest and lowest values were obtained for the DEC + 1-ol and DEC + 2,2-ol systems respectively. This could be because the linear alcohol molecules, such as 1-ol, show higher intermolecular interactions (dispersion forces) than those that show the branched-chain alcohols, such as 2,2-ol [96].

The $\delta\sigma$ of all systems studied in this work show negative values except for the DEC + 1-ol, DEC + 2-ol, and DEC + 3,2-ol systems, which present a sigmoidal curve. In the case of 1-ol and 2-ol positive values are observed for rich concentrations of DEC ($x_{DEC} > 0.8$) while for 3,2-ol positive values are obtained at low carbonate mole fractions ($x_{DEC} <$
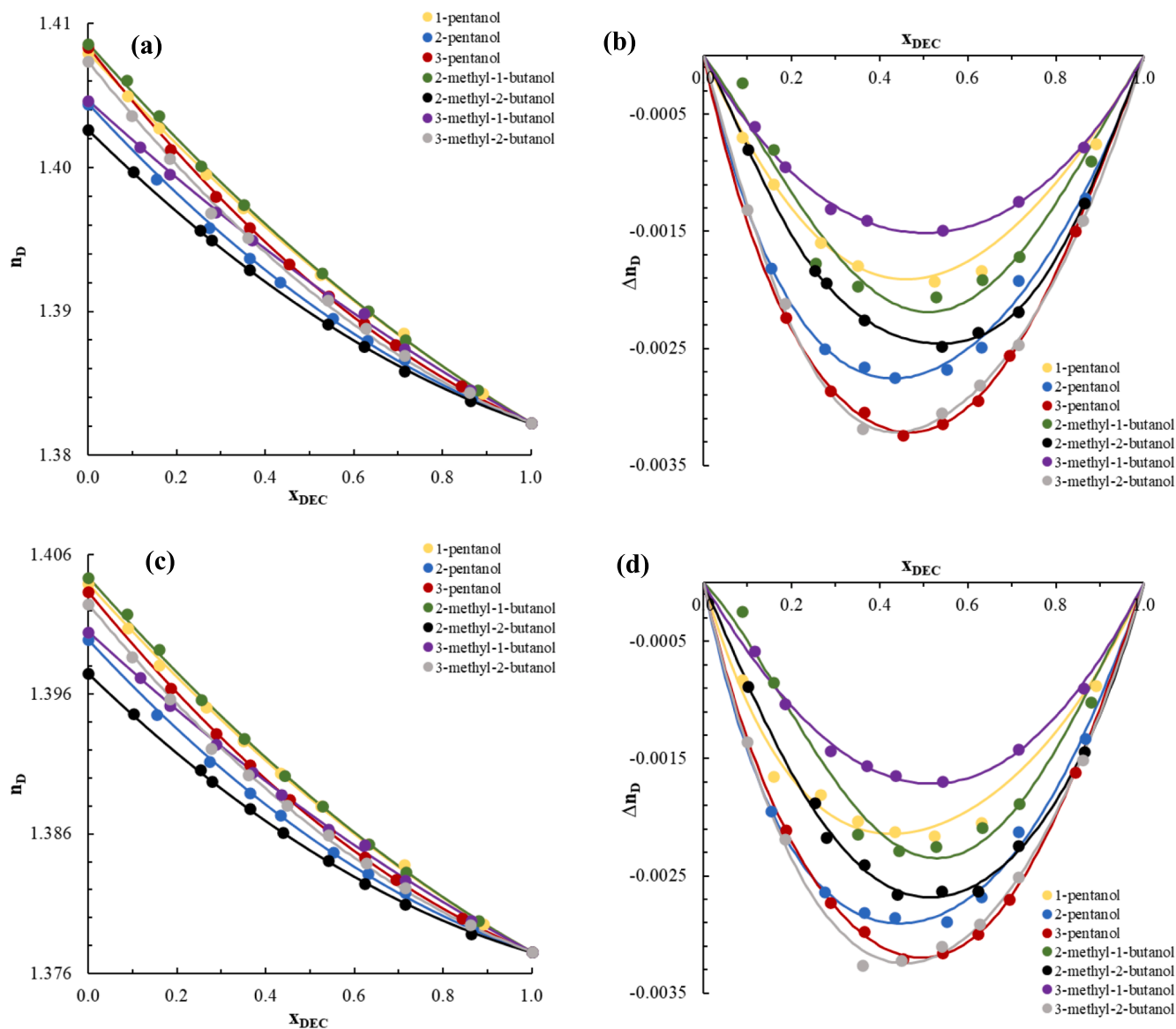
Fig. 4. Refractive indexes and changes in the refractive index of DEC + pentanol isomers (a) and (b) at 298.15 K and (c) and (d) at 308.15 K. The continuous lines in the refractive indexes correspond to a polynomial fit. The continuous lines in the changes in the refractive index correspond to the fit of a Redlich-Kister equation (Eq. (5)).

0.2). If we analyse the order of the δ σ, the maximum values −0.17 and −0.41 mN·m^{-1} are found towards carbonate-rich mole fractions ($x_{DEC} \approx$ 0.6). The values obtained for the different isomers, in absolute value, are as follows 2,2-ol > 3-ol > 3,2-ol > 1-ol > 2,1-ol > 2-ol > 3,1-ol, being the highest values obtained for the DEC + 2,2-ol mixture due to the great difference that exist between the surface tension of their pure components but it should be noted, that the values of both carbonate and pentanols are very similar and this does not allow any conclusion to be drawn.

The measured refractive index values and the calculated changes in the refractive index are shown in Fig. 4 (Table S3), where in (a) and (b) DEC + pentanol isomers at 298.15 K and in (c) and (d) DEC + pentanol isomers at 308.15 K. The refractive indexes are fitted to a Redlich-Kister type equation (Eq. (5) whose parameters are given in Table 3. As shown in Fig. 4 (a) and (c) the refractive indexes decrease nonlinearly with the increase of carbonate concentration.

The refractive index value is a measure of molecular electronic polarizability and its variation with concentration provides information

on the London dispersion forces of the molecules [52].

All the systems studied in this work at both temperatures show negative values of the change in the refractive indexes, that means that dispersion forces between the components of the mixtures are weaker than those of the pure components.

The behaviour of the isomers of pentanol, in absolute value, is the same at both temperatures 3-ol ≈ 3,2-ol > 2-ol > 2,2-ol > 2,1-ol > 1-ol > 3,1-ol. Thus, the highest and the lowest values are obtained for the secondary and primary alcohols respectively. The maximum values of the changes in the refractive indexes −0.0032 y − 0.0015 are shifted to fraction molar of DEC of 0.36 and 0.55 at the temperatures 298.15 K and 308.15 K. As can be seen we found little differences between the values obtained to both temperatures.

Previously, DEC + 1-pentanol values at 298.15 K have been published [31]. Comparing our refractive indexes with those published the difference of 0.05 % between the results is observed. In the case of the changes in the refractive index the difference found was of 10 %.

The derived excess functions of the binary systems were fitted by a

Table 4

Standard deviations, s, of the surface tension deviations, $\delta \sigma$, (mN·m^{-1}) from the predicted ones using the HSIS, HSEG, and Sugden equations.

	HSIS	HSEG	Sugden
DEC + 1-pentanol	0.13	0.11	0.13
DEC + 2-pentanol	0.05	0.08	0.33
DEC + 3-pentanol	0.23	0.26	0.30
DEC + 2-methyl-1-butanol	0.11	0.14	0.14
DEC + 2-methyl-2-butanol	0.29	0.35	0.04
DEC + 3-methyl-1-butanol	0.01	0.05	0.11
DEC + 3-methyl-2-butanol	0.12	0.15	0.29

Redlich-Kister type equation which was optimized by applying the F-test [97,98]

$$Q_{12}^E = x_1 x_2 \sum_{k=0}^{m} A_k (2x_1 - 1)^k \tag{5}$$

where Q_{12}^E represents H_m^E, V_m^E, $\Delta\eta$, $\delta\sigma$ or Δn_D. The coefficients A_k of the equation (5) and the standard deviations, s, defined by equation (6), are given in Table 3.

$$s = \sqrt{\frac{\sum_{i=1}^{N} \left(Y_{cal} - Y_{exp}\right)^2}{N - 1}} \tag{6}$$

where N is the number of data points, Y_{cal} the calculated value and Y_{exp} the experimental value.

In addition, we compare our values of surface tension with those obtained from the theoretical models of Hildebrand and Scott (HSIS, HSEG) and Sugden.

The HSIS model [99] is based on Guggenheim's ideal solution equation [100]. It applies when the size of the molecules in the mixture is similar and assumes that both the bulk liquid and the surface layer form ideal solutions. The equation for HSIS model can be written as:

$$\delta\sigma = -\frac{A_x}{2RT}(\sigma_1 - \sigma_2)^2 x_1 (1 - x_1) \tag{7}$$

where $\delta\sigma$ is the surface tension deviation, x_1 the mole fraction of DEC, σ_1 and σ_2 the surface tension of pure components, DEC and pentanol isomers respectively (Table 2), R the gas constant, T the temperature and A_x the molar surface area which will be defined as

$$A_x = x_1 A_1 + x_2 A_2 \tag{8}$$

The molar surface area of the pure compounds can be defined using different expressions [101–104] for our case we will use the most usual expression [101,103], which assumes that molecules in the liquid are close-packed spheres:

$$A_i = \left(V_i^2 \bullet N\right)^{1/3} \tag{9}$$

where N is Avogadro's number and V_i is the molecular volume of compound i that is obtained experimentally from their molecular mass and density. The standard deviations, s, defined by equation (6), are given in Table 4.

Another of the models applied is the HSEG which like the previous model is based on Guggenheim's ideal solution equation [100] but considering the different sizes of the molecules of the mixture. The expression for σ in the HSEG model can be written as [99,105]:

$$\sigma = Y_1\sigma_1 + Y_2\sigma_2 - \frac{(\sigma_1 - \sigma_2)^2}{2RT}(Y_1 A_1 + Y_2 A_2)Y_1 Y_2 \tag{10}$$

In this expression, the parameter Y_i gives the relationship between the surface molar area for the molecule i and the total molar surface area. Thus, Y_i is defined by the following expression:

$$Y_i = \frac{x_i A_i}{x_1 A_1 + x_2 A_2} \tag{11}$$

Note that in equation (10) we have changed the original Boltzmann's constant k_B into the gas constant R. This is because in original papers [99,105] A_i indicates the molecular surface area, but we will use the molar surface area defined in equation (9). To obtain $\delta\sigma$ we applied equation (3) to the σ values obtained from equation (10). The standard deviations, s, were calculated with equation (6) and showed in Table 4.

Finally, we analysed the theoretical model of Sugden [106] where a parameter called parachor is defined as:

$$[P_i] = \sigma_i^{1/4} \frac{M_i}{\rho_i} \tag{12}$$

M_i is the molar mass of the pure compound i, ρ_i its density and $[P_i]$ is the parachor which is independent of the temperature and characteristic of any liquid substance. This equation assumes that vapour density is negligible, which is the case of our measurements. Assuming that the parachor is mole-wise additive [95] we could define σ for a binary mixture as

$$\sigma = \left\{ [P_1]\frac{x_1}{M_m} + [P_2]\frac{1 - x_1}{M_m} \right\}^4 \rho^4 \tag{13}$$

$[P_1]$ and $[P_2]$ are the parachor coefficients for, respectively, DEC (1) and pentanol isomers (2), M_m and ρ are the molar mass and the density of the mixture. Once we know the parachor of the pure compounds (equation (12) and the densities of the mixtures, it is possible to calculate a semiempirical surface tension for any mixture. The standard deviations of the surface tension deviations were calculated with equation (6), these values are shown in Table 4.

In general, the best results are obtained for the HSIS theory due to the similarity of the size of the molecules of our systems. For the HSIS and HSEG, the system DEC + 3,1-ol is that which obtained the smallest standard deviation.

Finally, we have tested five empirical models to predict n_D from the density and n_D values of their pure compounds. These models are those of Lorentz-Lorenz (L-L), Wiener (W), Heller (H), Gladstone-Dale (G-D) and Newton (N).

The Lorentz-Lorenz equation [107,108] is defined as

$$\frac{n_{12}^2 - 1}{n_{12}^2 + 2} = \phi_1\left(\frac{n_1^2 - 1}{n_1^2 + 2}\right) + \phi_2\left(\frac{n_2^2 - 1}{n_2^2 + 2}\right) \tag{14}$$

being n_1 and n_2 the refractive indexes of the DEC and pentanol isomers, respectively, the n_{12} the refractive index of the mixture and ϕ is defined by the following equation:

$$\phi_i = w_i \frac{\rho_{12}}{\rho_i} \tag{15}$$

where ρ_{12} is the density of the mixture, ρ_i is the density of component i and w_i is the mass fraction of component i given by the following expression:

$$w_i = \frac{x_i M_i}{x_1 M_1 + x_2 M_2} \tag{16}$$

where x_i and M_i are the mole fraction and molar mass of component i, being DEC (1) and the pentanol isomers (2).

The expression of Wiener [109] that can be written as

$$\frac{n_{12}^2 - n_1^2}{n_{12}^2 + 2n_1^2} = \phi_2\left(\frac{n_2^2 - n_1^2}{n_2^2 + 2n_1^2}\right) \tag{17}$$

The next model applied was the Heller model [110]:

$$\frac{n_{12} - n_1}{n_1} = \frac{3}{2}\phi_2\left(\frac{m^2 - 1}{m^2 + 2}\right) \tag{18}$$

where m is calculated by the following expression:

$$m = \frac{n_2}{n_1} \tag{19}$$

Table 5

Standard deviations, s, of the experimental n_D results from the predicted ones using the Lorentz-Lorenz (L-L), Wiener (W), Heller (H), Gladstone-Dale (G-D) and Newton (N) equations.

	L-L	W	H	G-D	N
T = 298.15 K					
DEC + 1-pentanol	0.0004	0.0009	0.0009	0.0002	0.0002
DEC + 2-pentanol	0.0004	0.0019	0.0019	0.0004	0.0005
DEC + 3-pentanol	0.0005	0.0021	0.0021	0.0002	0.0003
DEC + 2-methyl-1-butanol	0.0004	0.0010	0.0010	0.0003	0.0003
DEC + 2-methyl-2-butanol	0.0002	0.0016	0.0016	0.0001	0.0003
DEC + 3-methyl-1-butanol	0.0002	0.0007	0.0007	0.0002	0.0002
DEC + 3-methyl-2-butanol	0.0003	0.0021	0.0021	0.0003	0.0005
T = 308.15 K					
DEC + 1-pentanol	0.0005	0.0011	0.0011	0.0004	0.0004
DEC + 2-pentanol	0.0006	0.0020	0.0020	0.0004	0.0005
DEC + 3-pentanol	0.0009	0.0021	0.0021	0.0005	0.0001
DEC + 2-methyl-1-butanol	0.0010	0.0011	0.0011	0.0007	0.0005
DEC + 2-methyl-2-butanol	0.0004	0.0018	0.0018	0.0002	0.0002
DEC + 3-methyl-1-butanol	0.0008	0.0008	0.0008	0.0006	0.0004
DEC + 3-methyl-2-butanol	0.0005	0.0022	0.0021	0.0002	0.0004

The Gladstone-Dale equation [111] has the form:

$$n_{12} - 1 = \phi_1(n_1 - 1) + \phi_2(n_2 - 1) \tag{20}$$

Finally, we applied the empirical expression known as Newton's equation [112], which is quite like that of Gladstone-Dale

$$n_{12}^2 = \phi_1\left(n_1^2 - 1\right) + \phi_2\left(n_2^2 - 1\right) + 1 \tag{21}$$

In Table 5, we give the standard deviations, s, (calculated with equation (6)) for the empirical models applied at temperatures 298.15 and 308.15 K. As can be seen, in general, the best prediction is given by Gladstone-Dale and Newton's equations and the empirical models of Wiener and Heller give very poor accuracy compared with the others, although their standard deviations are similar. In conclusion, the models of Gladstone-Dale and Newton could be used to estimate reliable n_{12} data for other similar mixtures from the data of n_1, n_2 and ρ_{12}.

4. Conclusions

In this work, we studied the physical properties of the mixtures the carbonate (DMC and DEC) with different isomers of pentanol and their deviation from the ideal behaviour through their corresponding excess magnitudes. Analaysing these latter properties, we set out to establish a relationship of the values obtained with the position of the —OH on the different isomers of pentanol. Thus, the results of the different excess properties (H_m^E, V_m^E, >0 and $\Delta\eta$, $\Delta\sigma$, $\Delta n_D < 0$) not only indicated that the interactions of the like molecules are stronger that of unlike molecules but also the steric effects including the free volume effects have an important impact on the interactions of the unlike ones in the mixing process. Thus, and taking into account that the isomers of pentanol have similar dipolar moments but different geometry, it was difficult to determine the influence of the position of the —OH in the obtained results.

The increase of the temperature provokes a decrease in viscosities and refractive indexes, although in these latter this increase is insignificant.

In general, at 298.15 K the mixtures with 1-ol and 3,1-ol (where the OH is on a primary carbon) show the best results for all studied properties.

Several theoretical models were applied to these systems for the surface tensions (HSIS, HSEG and Sugden) and the refractive indexes (Lorentz-Lorenz, Wiener, Heller, Gladstone-Dale and Newton). The best results were obtained for the model of HSIS in the case of surface tensions and the Gladstone-Dale and Newton for the refractive indexes.

CRediT authorship contribution statement

Montserrat Domínguez-Pérez: Conceptualization, Formal analysis, Investigation, Writing – original draft, Writing – review & editing, Data curation. **Luisa Segade:** Formal analysis. **Oscar Cabeza:** Formal analysis, Writing – review & editing. **Pablo Ligero:** Formal analysis. **Sandra García-Garabal:** Conceptualization, Formal analysis, Investigation, Writing – original draft, Writing – review & editing, Data curation.

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.

Data availability

I have shared my data at the Attach File step in Supplementary Material

Appendix A. Supplementary material

Supplementary data to this article can be found online at https://doi.org/10.1016/j.molliq.2023.122516.

References

[1] N. Winterton, The green solvent: a critical perspective, Clean Techn. Environ. Policy 23 (2021) 2499–2522, https://doi.org/10.1007/s10098-021-02188-8.

[2] C.J. Clarke, W.-C. Tu, O. Levers, A. Bröhl, J.P. Hallett, Green and sustainable solvents in chemical processes, Chem. Rev. 118 (2018) 747–800, https://doi.org/10.1021/acs.chemrev.7b00571.

[3] H. Mutlu, L. Barner, Getting the terms right: green, sustainable, or circular chemistry? Macromol. Chem. Phys. 223 (2022), 2200111 https://doi.org/10.1002/macp.202200111.

[4] M.A. Rasool, P.P. Pescarmona, I.F.J. Vankelecom, Applicability of organic carbonates as green solvents for membrane preparation, ACS Sustain. Chem. Eng. 7 (2019) 13774–13785, https://doi.org/10.1021/acssuschemeng.9b01507.

[5] D. Ho, J. Lee, S. Park, Y. Park, K. Cho, F. Campana, D. Lanari, A. Facchetti, S.Y. Seo, C. Kim, A. Marrocchi, L. Vaccaro, Green solvents for organic thin-film transistor processing, J. Mater. Chem. C 8 (2020) 5786–5794, https://doi.org/10.1039/D0TC00512F.

[6] L.D. Almeida, F.G. Delolo, A.P.S. Costa, E.V. Gusevskaya, P.A. Robles-Azocar, Catalytic aerobic epoxidation of bio-renewable alkenes using organic carbonates as green solvents, Mol. Catal. 527 (2022), 112400, https://doi.org/10.1016/j.mcat.2022.112400.

[7] A.O.G. Abdalla, D. Liu, Dimethyl carbonate as a promising oxygenated fuel for combustion: a review, Energies 11 (2018), 1552, https://doi.org/10.3390/en11061552.

[8] X. Liu, D. Xu, B. Diao, L. Zhang, J. Gao, D. Liu, Y. Wang, Choline chloride based deep eutectic solvents selection and liquid-liquid equilibrium for separation of dimethyl carbonate and ethanol, J. Mol. Liq. 275 (2019) 347–353, https://doi.org/10.1016/j.molliq.2018.11.047.

[9] P. Tundo, M. Musolino, F. Aricò, The reactions of dimethyl carbonate and its derivatives, Green Chem. 20 (2018) 28–85, https://doi.org/10.1039/C7GC01764B.

[10] S. Prati, G. Sciutto, F. Volpi, C. Rehorn, R. Vurro, B. Blümich, L. Mazzocchetti, L. Giorgini, C. Samorì, P. Galletti, E. Tagliavini, R. Mazzeo, Cleaning oil paintings: NMR relaxometry and SPME to evaluate the effects of green solvents and innovative green gels, New J. Chem. 43 (2019) 8229–8238, https://doi.org/10.1039/C9NJ00186G.

[11] A. Ismael, A. Gevorgyan, T. Skrydstrup, A. Bayer, Renewable solvents for palladium-catalyzed carbonylation reactions, Org. Process Res. Dev. 24 (2020) 2665–2675, https://doi.org/10.1021/acs.oprd.0c00325.

[12] O. Gómez-de-Miranda-Jiménez-de-Aberasturi, A. Centeno-Pedrazo, S. Prieto Fernández, R. Rodriguez Alonso, S. Medel, J.M. Cuevas, L.G. Monsegue, S. De Wildeman, E. Benedetti, D. Klein, H. Henneken, J.R. Ochoa-Gómez, The future of isosorbide as a fundamental constituent for polycarbonates and polyurethanes, Green Chem. Lett. Rev. 14 (2021) 534–544, https://doi.org/10.1080/17518253.2021.1965223.

[13] A. Hofmann, Z. Wanga, S. Pinto Bautista, M. Weil, F. Müller, R. Löwe, L. Schneider, I. UlMohsin, T. Hanemann, Comprehensive characterization of propylene carbonate based liquid electrolyte mixtures for sodium-ion cells, Electrochim. Acta 403 (2022), 139670, https://doi.org/10.1016/j.electacta.2021.139670.

[14] J. Tong, X. Xiao, X. Liang, N. von Solms, F. Huo, H. He, S. Zhang, Insights into the solvation and dynamic behaviors of a lithium salt in organic- and ionic liquid-based electrolytes, PCCP 21 (2019) 19216–19225, https://doi.org/10.1039/C9CP01848D.

[15] Y. Huang, H. Wang, Cooperation of dimethyl and diethyl carbonates in hexafluorophosphate anion intercalation into graphite electrode, Langmuir 36 (2020) 9909–9915, https://doi.org/10.1021/acs.langmuir.0c01593.

[16] S. Choudhury, Lithium Fluoride Additives for Stable Cycling of Lithium Batteries at High Current Densities, Rational Design of Nanostructured Polymer Electrolytes and Solid-Liquid Interphases for Lithium Batteries, Springer Theses. Springer, Cham, 2019, pp. 81–94.

[17] W. Wahyudi, V. Ladelta, L. Tsetseris, M.M. Alsabban, X. Guo, E. Yengel, H. Faber, B. Adilbekova, A. Seitkhan, A.-H. Emwas, M.N. Hedhili, L.-J. Li, V. Tung, N. Hadjichristidis, T.D. Anthopoulos, J. Min, Lithium-ion desolvation induced by nitrate additives reveals new insights into high performance lithium batteries, Adv. Funct. Mater. 31 (2021), 2101593, https://doi.org/10.1002/adfm.202101593.

[18] X. Cao, H. Jia, W. Xu, J.-G. Zhang, Review—Localized high-concentration electrolytes for lithium batteries, J. Electrochem. Soc. 168 (2021), 010522, https://doi.org/10.1149/1945-7111/abd60e.

[19] M. Yabré, L. Ferey, I.T. Somé, K. Gaudin, Greening reversed-phase liquid chromatography methods using alternative solvents for pharmaceutical analysis, Molecules 23 (2018), 1065, https://doi.org/10.3390/molecules23051065.

[20] Y. Yoshimoto, E. Tserenochir, E. Kinoshita, T. Otaka, Combustion improvements by C4/C5 bio-alcohol isomer blended fuels combined with supercharging and EGR in a diesel engine, World Acad. Sci. Eng. Technol. Int. J. Mech. Mechatron. Eng. 12 (2019) 961–969, ISNI: 0000000091950263.

[21] C. Cao, Y. Zhang, X. Zhang, J. Zou, F. Qi, Y. Li, J. Yang, Experimental and kinetic modeling study on flow reactor pyrolysis of iso-pentanol: understanding of iso-pentanol pyrolysis chemistry and fuel isomeric effects of pentanol, Fuel 257 (2019), 116039, https://doi.org/10.1016/j.fuel.2019.116039.

[22] L.T. Vargas-Ibáñez, J.J. Cano-Gómez, G.A. Iglesias-Silva, I.A. Santos-López, O. E. Benavides-Moran, P. Zwolinski, Physical properties of biodiesel blended with hexanol isomers at different temperatures: surface tension, density, viscosity, and refractive index, J. Chem. Eng. Data 65 (2020) 3706–3727, https://doi.org/10.1021/acs.jced.0c00328.

[23] J. Fabbria, C.M. Clemente, N. Elissondo, G. Gambino, S. Ravetti, L.Y. Hergert, S. D. Palma, M.C. Elissondo, Anti-echinococcal activity of menthol and a novel prodrug, menthol-pentanol, against *Echinococcus multilocularis*, Acta Trop. 205 (2020), 105411, https://doi.org/10.1016/j.actatropica.2020.105411.

[24] L.T. Vargas-Ibáñez, J.J. Cano-Gómez, I.A. Santos-López, G.A. Iglesias-Silva, J. S. López-Lázaro, M.M. Alcalá-Rodríguez, C. Villarreal-Mendoza, C. Armendáriz-Ovalle, Surface tensions of biodiesel blends with pentanol and octanol isomers at different conditions: measurement and new correlation, Fluid Phase Equilib. 540 (2021), 113046, https://doi.org/10.1016/j.fluid.2021.113046.

[25] A. Lestido-Cardama, P. Vázquez Loureiro, R. Sendón, P. Paseiro Losada, A. Rodríguez Bernaldo de Quirós, Application of chromatographic analysis for detecting components from polymeric can coatings and further determination in beverage samples, J. Chromatogr. A 1638 (2021), 461886, https://doi.org/10.1016/j.chroma.2021.461886.

[26] S. Verma, S. Gahlyan, M. Rani, S. Maken, Excess molar enthalpies of n-alkanol (C2–C10) with n-decane at 298.15 K: Flory–Treszczanowicz–Benson model, J. Mol. Liq. 265 (2018) 468–472, https://doi.org/10.1016/j.molliq.2018.06.046.

[27] S. Verma, S. Gahlyan, J. Kaur, S. Maken, Excess enthalpy of ethanol + n-alkane (C6–C9) or cyclohexane or diisopropyl ether mixtures at 298.15 K: Measurement and modeling, J. Mol. Liq. 292 (2019), 111359, https://doi.org/10.1016/j.molliq.2019.111359.

[28] R. Francesconi, F. Comelli, C. Castellari, Excess molar enthalpies of diethyl carbonate + seven pentanol isomers at 298.15 K. Use of the extended cell model of Prigogine, Thermochim Acta 327 (1999) 145–149, https://doi.org/10.1016/S0040-6031(98)00600-5.

[29] C. Yang, H. Lai, Z. Liu, P. Ma, Density and viscosity of binary mixtures of diethyl carbonate with alcohols at (293.15 to 363.15) K and predictive results by UNIFAC-VISCO group contribution method, J. Chem. Eng. Data 51 (2006) 1345–1351, https://doi.org/10.1021/je0600808.

[30] A. Rodríguez, J. Canosa, A. Domínguez, J. Tojo, Dynamic viscosities of diethyl carbonate with linear and secondary alcohols at several temperatures, J. Chem. Eng. Data 49 (2004) 157–162, https://doi.org/10.1021/je0341413.

[31] A. Rodríguez, J. Canosa, J. Tojo, Density, Refractive index, and speed of sound of binary mixtures (diethyl carbonate + alcohols) at several temperatures, J. Chem. Eng. Data 46 (2001) 1506–1515, https://doi.org/10.1021/je010148d.

[32] A. Rodríguez, J. Canosa, J. Tojo, Physical properties of binary mixtures (dimethyl carbonate + alcohols) at several temperatures, J. Chem. Eng. Data 46 (2001) 1476–1486, https://doi.org/10.1021/je0101193.

[33] M. Almasi, Thermodynamic properties of binary mixtures containing dimethyl carbonate+2-alkanol: experimental data, correlation and prediction by ERAS model and cubic EOS, Phys. B Condens. Matter 412 (2013) 100–105, https://doi.org/10.1016/j.physb.2012.12.005.

[34] P.V. Verdes, M.M. Mato, M.I. Paz Andrade, J.L. Legido, Contribution to study of the thermodynamics properties of mixtures containing 2-methoxy-2-

[35] methylpropane, alkanol, alkane, J. Chem. Thermodyn. 73 (2014) 224–231, https://doi.org/10.1016/j.jct.2014.01.002.

[35] O. Cabeza, J. Vila, E. Rilo, M. Domínguez-Pérez, L. Otero-Cernadas, E. López-Lago, T. Méndez-Morales, L.M. Varela, Physical properties of aqueous mixtures of the ionic 1-ethl-3-methyl imidazolium octyl sulfate: a new ionic rigid gel, J. Chem. Thermodyn. 75 (2014) 52–57, https://doi.org/10.1016/j.jct.2014.04.016.

[36] R. Miller, A. Hofmann, R. Hartmann, A. Halbig, K.-H. Schano, Measuring dynamic surface and interfacial tensions, Adv. Mater. 4 (1992) 370–374, https://doi.org/10.1002/adma.19920040513.

[37] S. García-Garabal, M. Domínguez-Pérez, D. Portela, L.M. Varela, O. Cabeza, Preliminary study of new electrolytes based on [MPPyr][TFSI] for lithium ion batteries, J. Mol. Liq. 363 (2022), 119758, https://doi.org/10.1016/j.molliq.2022.119758.

[38] J.M. Pardo, C.A. Tovar, C.A. Cerdeiriña, E. Carballo, L. Romaní, Excess quantities of dialkyl carbonate + cyclohexane mixtures at a variable temperature, Fluid Phase Equilib. 179 (2001) 151–163, https://doi.org/10.1016/S0378-3812(00)00491-X.

[39] J. Deng, Y. Yang, Y. He, G. Ouyang, Z. Huang, Densities and surface tensions of trimethylbenzene + dimethyl carbonate or + diethyl carbonate at 298.15 K and 313.15 K, J. Chem. Eng. Data 51 (2006) 1464–1468, https://doi.org/10.1021/je060137q.

[40] Y. Xing, W. Fang, D. Li, Y. Guo, R. Lin, Density, viscosity, and vapor pressure for binary mixtures of tricyclo [5.2.1.0$^{2.6}$] decane and diethyl carbonate, J. Chem. Eng. Data 54 (2009) 1865–1870, https://doi.org/10.1021/je800984q.

[41] H. Iloukhani, H.A. Zarei, M. Behroozi, Thermodynamic studies of ternary mixtures of diethylcarbonate (1) + dimethylcarbonate (2) + N, N-dimethylacetamide (3) at 298.15 K, J. Mol. Liq. 135 (2007) 141–145, doi: 10.1016/j.molliq.2006.11.009.

[42] Q. Liu, L. Zhao, Q. Zheng, L. Mou, P. Zhang, Excess molar volume and viscosity deviation of [C$_2$mim][NTf$_2$]/[C$_4$mim][NTf$_2$] + DMC/DEC, J. Chem. Eng. Data 63 (2018) 4484–4496, https://doi.org/10.1021/acs.jced.8b00591.

[43] L. Mou, Y. Chai, G. Yang, Q. Xia, Q. Liu, Q. Zheng, Q. Zhang, Density and viscosity of four binary mixtures of [C$_2$mmim][NTf$_2$]/[C$_4$mmim][NTf$_2$] + dimethyl carbonate/diethyl carbonate, J. Chem. Thermodyn. 130 (2019) 183–191, https://doi.org/10.1016/j.jct.2018.10.015.

[44] L. Mosteiro, L.M. Casás, J.L. Legido, Surface tension, density, and speed of sound for the ternary mixture {diethyl carbonate + p-xylene + decane}, J. Chem. Thermodyn. 41 (2009) 695–704, https://doi.org/10.1016/j.jct.2008.12.010.

[45] N.A. Lange (Ed.), Handbook of Chemistry, 15th ed., McGraw-Hill, New York, 1999.

[46] A. Rodríguez, J. Canosa, J. Tojo, Physical properties of the binary mixtures (diethyl carbonate + hexane, heptane, octane and cyclohexane) from T=293.15 K to T=313.15 K, J. Chem. Thermodyn. 35 (2003) 1321–1333, https://doi.org/10.1016/S0021-9614(03)00096-X.

[47] L. Mosteiro, E. Mascato, B.E. de Cominges, T.P. Iglesias, J.L. Legido, Density, speed of sound, refractive index and dielectric permittivity of (diethyl carbonate + n-decane) at several temperatures, J. Chem. Thermodyn. 33 (2001) 787–801, https://doi.org/10.1006/jcht.2000.0779.

[48] F. Comelli, R. Francesconi, A. Bigi, K. Rubini, Excess molar enthalpies, molar heat capacities, densities, viscosities, and refractive indices of dimethyl sulfoxide + esters of carbonic acid at 308.15 K and atmospheric pressure, J. Chem. Eng. Data 51 (2006) 665–670, https://doi.org/10.1021/je050444g.

[49] J. Troncoso, D. Bessières, C.A. Cerdeiriña, E. Carballo, L. Romaní, pρTx data for the dimethyl carbonate + decane system, J. Chem. Eng. Data 49 (2004) 923–927, https://doi.org/10.1021/je0342320.

[50] B.R. Arbad, M.K. Lande, N.N. Wankhede, D.S. Wankhede, Viscosities, ultrasonic velocities at (288.15 and 298.15) K, and refractive indices at (298.15) K of binary mixtures of 2,4,6-trimethyl-1,3,5-trioxane with dimethyl carbonate, diethyl carbonate, and propylene carbonate, J. Chem. Eng. Data 51 (2006) 68–72, https://doi.org/10.1021/je050183a.

[51] E. Romano, J.L. Trenzado, E. González, J.S. Matos, L. Segade, E. Jiménez, Thermophysical properties of four binary dimethyl carbonate + 1-alcohol systems at 288.15–313.15 K, Fluid Phase Equilib. 211 (2003) 219–240, doi: 10.1016/S0378-3812(03)00203-6.

[52] A.G. Gilani, A. Mirkhalili, Dielectric, volumetric, refractometric, and excess properties of (cycloalkanone + pentanol isomers) systems at T = 298.15 K, J. Chem. Eng. Data 66 (2021) 3934–3950, https://doi.org/10.1021/acs.jced.1c00545.

[53] C. Sharma, C. Bakshi, U. Syal, S. Devi, A.K. Sharma, M. Sharma, Addition of 1-pentanol, cyclopentanol, and 2-methyl-1-butanol as biofuels into jet fuel component (tridecane): excess thermodynamic and acoustic approach, J. Chem. Eng. Data 67 (2022) 1054–1069, https://doi.org/10.1021/acs.jced.2c00005.

[54] G.A. Iglesias-Silva, J.J. Cano-Gómez, L.T. Vargas-Ibáñez, H.J. Amezquita-Garcia, F.J. Cerino-Córdova, Densities and viscosities for binary liquid mixtures of pentanol isomers from (288.15 to 328.15) K at 0.1 MPa, J. Chem. Eng. Data 64 (2019) 1922–1936, doi: 10.1021/acs.jced.8b00979.

[55] N.V. Sastry, M.K. Valand, Viscosities and densities for heptane + 1-pentanol, +1-hexanol, +1-heptanol, +1-octanol, +1-decanol, and +1-dodecanol at 298.15 K and 308.15 K, J. Chem. Eng. Data 41 (1996) 1426–1428, https://doi.org/10.1021/je9601725.

[56] L. Segade, J. Jiménez de Llano, M. Domínguez-Pérez, O. Cabeza, M. Cabanas, E. Jiménez, Density, surface tension, and refractive index of octane + 1-alkanol mixtures at T = 298.15 K, J. Chem. Eng. Data 48 (2003) 1251–1255, https://doi.org/10.1021/je034053i.

[57] A.A. Rafati, E. Ghasemian, M. Abdolmaleki, Surface properties of binary mixtures of ethylene glycol with a series of aliphatic alcohols (1-pentanol, 1-hexanol, and 1-heptanol), J. Chem. Eng. Data 53 (2008) 1944–1949, https://doi.org/10.1021/je800101v.

[58] T.P. Iglesias, J.L. Legido, S.M. Pereira, B. de Cominges, M.I. Paz Andrade, Relative permittivities and refractive indices on mixing for (n-hexane + 1-pentanol, or 1-hexanol, or 1-heptanol) at T = 298.15 K, J. Chem. Thermodyn. 32 (2000) 923–930, https://doi.org/10.1006/jcht.2000.0661.

[59] M.S. Reddy, I. Khan, K.T.S.S. Raju, P. Suresh, B.H. Babu, The study of molecular interactions in 1-ethyl-3-methylimidazolium trifluoromethanesulfonate + 1-pentanol from density, speed of sound and refractive index measurements, J. Chem. Thermodyn. 98 (2016) 298–308, https://doi.org/10.1016/j.jct.2016.03.014.

[60] M. Lj. Kijevčanin, I.R. Radović, B.D. Djordjević, A.Ž. Tasić, S.P. Šerbanović, Experimental determination and modeling of densities and refractive indices of the binary systems alcohol + dicyclohexylamine at T = (288.15–323.15) K, Thermochim. Acta 525 (2011) 114–128, doi: 10.1016/j.tca.2011.08.002.

[61] S. Aznarez, M.M.E.F. de Ruiz Holgado, E.L. Arancibia, Viscosities of mixtures of 2-alkanols with tetraethyleneglycol dimethyl ether at different temperatures, J. Mol. Liq. 124 (2006) 78–83, doi: 10.1016/j.molliq.2005.09.003.

[62] A.F. Ribeiro, E. Langa, A.M. Mainar, J.I. Pardo, J.S. Urieta, Excess molar enthalpy, density, and speed of sound for the mixtures β-pinene + 1- or 2-pentanol at (283.15, 298.15, and 313.15) K, J. Chem. Eng. Data 51 (2006) 1846–1851, https://doi.org/10.1021/je060210c.

[63] S. Toshiomi, Dielectric dispersion and intermolecular association for 28 pure liquid alcohols. The position dependence of hydroxyl group in the hydrocarbon chain, Bull. Chem. Soc. Jpn. 62 (1989) 908–914, https://doi.org/10.1246/bcsj.62.908.

[64] L.T. Vargas-Ibáñez, G.A. Iglesias-Silva, J.J. Cano-Gómez, C. Escamilla-Alvarado, M.A. Berrones-Eguiluz, Densities and viscosities for binary liquid mixtures of biodiesel + 1-pentanol, 2-pentanol, or 2-methyl-1-butanol from (288.15 to 338.15) K at 0.1 MPa, J. Chem. Eng. Data 63 (2018) 2438–2450, https://doi.org/10.1021/acs.jced.7b00996.

[65] L.T. Vargas-Ibáñez, J.J. Cano-Gómez, I.A. Santos-López, G.A. Iglesias-Silva, J.S. López-Lázaro, M.M. Alcalá-Rodríguez, C. Villarreal-Mendoza, C. Armendáriz-Ovalle, Surface tensions of biodiesel blends with pentanol and octanol isomers at different conditions: measurement and new correlation, Fluid Phase Equilib. 540 (2021) 113046, doi: 10.1016/j.fluid.2021.113046.

[66] S. Azizian, N. Bashavard, Surface tension of dilute solutions of linear alcohols in benzyl alcohol, J. Chem. Eng. Data 50 (2005) 1303–1307, https://doi.org/10.1021/je0500431.

[67] H. Iloukhani, M. Soleimani, Measurement and modeling the excess molar volumes and refractive index deviations of binary mixtures of 2-propanol, 2-butanol and 2-pentanol with N-propylamine, J. Sol. Chem. 46 (2017) 2135–2158, https://doi.org/10.1007/s10953-017-0683-y.

[68] S. Akhtar, K.M.S. Hossain, M.A. Saleh, Viscosity and thermodynamics of viscous flow for the systems of isomeric pentanols with toluene, Phys. Chem. Liq. 40 (2002) 435–448, https://doi.org/10.1080/0031910021000017753.

[69] J.A. Riddick, W.B. Bunger, T.K. Sakano, Organic Solvents, Wiley Interscience, New York, 1986.

[70] M.-G. Kim, Ternary and constituent binary excess molar enthalpies of 1,2-dichloropropane + 2-pentanol + 3-pentanol at T=298.15K, Kor. J. Chem. Eng. 31 (2014) 315–321, https://doi.org/10.1007/s11814-013-0229-y.

[71] M. Almasi, H. Iloukhani, Densities, viscosities, and refractive indices of binary mixtures of methyl ethyl ketone + pentanol isomers at different temperatures, J. Chem. Eng. Data 55 (2010) 3918–3922, https://doi.org/10.1021/je901067c.

[72] M. Dzida, Study of the effects of temperature and pressure on the thermodynamic and acoustic properties of 2-methyl-1-butanol at temperatures from 293K to 318K and pressures up to 100MPa, Int. J. Thermophys. 31 (2010) 55–69, https://doi.org/10.1007/s10765-009-0607-1.

[73] J.M. Resa, J.M. Goenaga, J. Lanz, M. Iglesias, Vapor−Liquid equilibrium of binary mixtures containing ethyl acetate + 2-methyl-1-propanol and ethyl acetate + 2-methyl-1-butanol at 101.3 kPa, J. Chem. Eng. Data 51 (2006) 595–598, https://doi.org/10.1021/je050420+.

[74] J.M. Goenaga, A. Gayol, R.G. Concha, M. Iglesias, J.M. Resa, Effect of temperature on thermophysical properties of ethanol + aliphatic alcohols (C4–C5) mixtures, Monatshefte für Chemie - Chemical Monthly 138 (2007) 403–436, https://doi.org/10.1007/s00706-007-0623-4.

[75] E. Garcia-Pañeda, P. Guardado, A. Maestre, Limiting partial molar volumes of electrolytes in 2-methyl-2-butanol + water mixtures at 298.15 K, J. Sol. Chem. 33 (2004) 1277–1293, https://doi.org/10.1007/s10953-004-7140-4.

[76] C. Bradtmöller, S. Scholl, Proposal for a viscous test mixture—densities, viscosities, and vapor–liquid equilibrium data of the binary mixture 2-methyl-2-butanol + 2-methyl-1-propanol, J. Chem. Eng. Data 61 (2016) 272–285, https://doi.org/10.1021/acs.jced.5b00537.

[77] M. Fattahi, H. Iloukhani, Excess molar volume, viscosity, and refractive index study for the ternary mixture 2-methyl-2-butanol (1) + tetrahydrofuran (2) + propylamine (3) at different temperatures. Application of the ERAS-model and Peng–Robinson–Stryjek–Vera equation of state, J. Chem. Thermodyn. 42 (2010) 1335–1345, https://doi.org/10.1016/j.jct.2010.05.009.

[78] J. Canosa, A. Rodríguez, J. Tojo, Dynamic viscosities of the binary mixtures (methyl acetate or methanol + 2-methyl-2-butanol) and the ternary mixtures (methyl acetate + methanol + 2-propanol, or 2-butanol, or 2-methyl-2-butanol) at T = 298.15 K, J. Chem. Thermodyn. 32 (2000) 551–565, https://doi.org/10.1006/jcht.2000.0628.

[79] H. Kumar, N. Gulati, V. Kundi, Viscometric studies of binary liquid mixtures of cyclopentane (1) + branched alkanols (2) at T = (298.15 and 308.15) K, J. Mol. Liq. 174 (2012) 63–69, doi: 10.1016/j.molliq.2012.07.020.

[80] E. Álvarez, A. Cancela, R. Maceiras, J.M. Navaza, R. Táboas, Density, viscosity, excess molar volume, and viscosity deviation of three amyl alcohols + ethanol binary mixtures from 293.15 to 323.15 K, J. Chem. Eng. Data 51 (2006) 940–945, https://doi.org/10.1021/je050416y.

[81] M. Dzida, P. Góralski, Molar heat capacities for (2-methyl-2-butanol + heptane) mixtures and cyclopentanol at temperatures from (284 to 353) K, J. Chem. Thermodyn. 41 (2009) 402–413, https://doi.org/10.1016/j.jct.2008.10.010.

[82] H. Iloukhani, K. Khanlarzadeh, Experimental study on the calorimetric data of butylacetate with pentanol isomers as important biofuels and correlation treatment at T = 298.15 K, Phys. Chem. Liq. 53 (2015) 559–573, https://doi.org/10.1080/00319104.2013.802207.

[83] J.M. Resa, C. González, M. Juez, S. Ortiz de Landaluce, Density, refractive index and speed of sound for mixtures of ethyl acetate with 2-butanol and 3-methyl-1-butanol: Vapor–liquid equilibrium of the ethyl acetate + 3-methyl-1-butanol system, Fluid Phase Equilib. 217 (2004) 175–180, https://doi.org/10.1016/j.fluid.2003.02.001.

[84] D.M. Bajić, E.M. Živković, S.S. Šerbanović, M.L. Kijevčanin, Volumetric and viscometric study of binary systems of ethyl butyrate with alcohols, J. Chem. Eng. Data 59 (2014) 3677–3690, https://doi.org/10.1021/je5005752.

[85] R. Tahery, Correlation between molecular sizes of pure compounds: application in surface tension prediction based on scaled particle theory, Adv. J. Chem.-Sect. A 4 (2021) 104–114, https://doi.org/10.22034/ajca.2021.271237.1237.

[86] T.M. Aminabhavi, S.K. Raikar, A study on mixing properties of binary mixtures of bromoform with aliphatic alcohols, J. Chem. Eng. Data 38 (1993) 310–319, https://doi.org/10.1021/je00010a033.

[87] W.-L. Weng, L.-T. Chang, I.-M. Shiah, Viscosities and densities for binary mixtures of benzylamine with 1-pentanol, 2-pentanol, 2-methyl-1-butanol, 2-methyl-2-butanol, 3-methyl-1-butanol, and 3-methyl-2-butanol, J. Chem. Eng. Data 44 (1999) 994–997, https://doi.org/10.1021/je990031d.

[88] A.G. Gilani, F. Amouzadeh, T. Taki, A comparative study on liquid phase equilibria of aqueous mixtures of two structurally close carboxylic acids with sec-amyl alcohols at 298.2 K, J. Mol. Liq. 324 (2021), 114733, https://doi.org/10.1016/j.molliq.2020.114733.

[89] J.A. González, F. Hevia, C. Alonso-Tristán, I. García de la Fuente, J.C. Cobos, Orientational effects in mixtures of organic carbonates with alkanes or 1-alkanols, Fluid Phase Equilib. 449 (2017) 91–103, https://doi.org/10.1016/j.fluid.2017.06.012.

[90] S. García-Garabal, L. Segade, M. Domínguez-Pérez, M. Cabanas, S. Yañez-Vilar, O. Cabeza, Excess molar enthalpies of the binary systems:(Dibutyl ether+ isomers of pentanol) at T = (298.15 and 308.15) K, J. Chem. Thermodyn. 87 (2015) 52–57, https://doi.org/10.1016/j.jct.2015.03.021.

[91] J.L. Trenzado, E. Romano, L. Segade, M.N. Caro, E. González, S. Galván, Densities and viscosities of four binary diethyl carbonate + 1-alcohol systems from (288.15 to 313.15) K, J. Chem. Eng. Data 56 (2011) 2841–2848, https://doi.org/10.1021/je1013476.

[92] A.A. Touazi, S. Didaoui, K. Khimeche, M. Rial, S.A. Moulaï, M. Benziane, Experimental and theoretical studies of volumetric and viscous properties of n-tetradecane with isomeric pentanols, J. Mol. Liq. 327 (2021), 114860, https://doi.org/10.1016/j.molliq.2020.114860.

[93] E.D. Dikio, I. Bahadur, E.E. Ebenso, Intermolecular interactions between 2-methyl-2-butanol and petroleum ether at different temperatures: density, viscosity and refractive index measurements, J. Mol. Liq. 219 (2016) 795–800, https://doi.org/10.1016/j.molliq.2016.04.041.

[94] R. Alcalde, M. Atilhan, J.L. Trenzado, S. Aparicio, Physicochemical insights on alkylcarbonate–alkanol solutions, J. Phys. Chem. B 120 (2016) 5015–5028, https://doi.org/10.1021/acs.jpcb.6b02961.

[95] R.C. Reid, J.M. Prausnitz, B.E. Poling, The Properties of Gases and Liquids, McGraw-Hill, New York, 1987.

[96] D. Zhao, Y. Zhuang, C. Fan, F. Yang, Y. Chen, X. Zhang, Surface tension of binary mixtures composed of N, N-dimethylcyclohexylamine and alcohols at different temperatures, J. Chem. Thermodyn. 143 (2020), 106041, https://doi.org/10.1016/j.jct.2019.106041.

[97] O. Redlich, A.T. Kister, Ind. Eng. Chem. 40 (1948) 341–345. 10.1021/ie50458a035.

[98] P.R. Bevington, D.K. Robinson, Data Reduction and Error Analysis for the Physical Sciences, 2nd ed., McGraw-Hill, Singapore, 1994.

[99] J.H. Hildebrand, R.L. Scott, Solubility of Nonelectrolytes, Reinhold Pub. Corp., New York, 1950.

[100] E.A. Guggenheim, Mixtures, Oxford University Press, London, 1950. Chapter 9.

[101] T.P. Hoar, D.A. Melford, The surface tension of binary liquid mixtures: lead + tin and lead + indium alloys, Trans. Faraday Soc. 53 (1957) 315–326, https://doi.org/10.1039/TF9575300315.

[102] S. Nath, Surface tension of nonideal binary liquid mixtures as a function of composition, J. Colloid Interf. Sci. 209 (1999) 116–122, https://doi.org/10.1006/jcis.1998.5873.

[103] S.K. Suri, V. Ramakrishna, Surface tension of some binary liquid mixtures, J. Phys. Chem. 72 (1968) 3073–3079, https://doi.org/10.1021/j100855a001.

[104] J. Tojo, C. Torres-Marchal, P. Rasmussen, Prediction of surface tensions of nonelectrolyte solutions, Chem. Eng. Sci. 44 (1989) 782–786.

[105] R.L. Schmidt, J.C. Randall, H.L. Clever, The surface tension and density of binary hydrocarbon mixtures: benzene-n-hexane and benzene-n-dodecane, J. Phys. Chem. 70 (1966) 3912–3916, https://doi.org/10.1021/j100884a027.

[106] S. Sugden, A relation between surface tension, density, and chemical composition, J. Chem. Soc. 125 (1924) 1177–1181, https://doi.org/10.1039/CT9242501177.

[107] H.A. Lorentz, Über die Beziehungzwischen der Fortpflanzungsgeschwindigkeit des Lichtes der Körperdichte, Ann. Phys. 9 (1880) 641–665, https://doi.org/10.1002/andp.18802450406.

[108] L. Lorenz, Über die Refractionsconstante, Ann. Phys. 11 (1880) 70–103, https://doi.org/10.1002/andp.18802470905.

[109] O. Wiener, Theory of refraction constants, Ber. Sächs. Ges. Wiss. 62 (1910) 256–277.

[110] W. Heller, The determination of refractive indices of colloidal particles by means of a new mixture rule or from measurements of light scattering, Phys. Rev. 68 (1945) 5–10, https://doi.org/10.1103/PhysRev.68.5.

[111] J.H. Gladstone, T.P. Dale, Researches on the refraction, dispersion, and sensitiveness of liquids, Philos. Trans. R. Soc. Lond. 153 (1863) 317–343. https://www.jstor.org/stable/108799.

[112] S.S. Jr, A.L.W. Kurtz, The refractivity intercept and the specific refraction equation of Newton. I. development of the refractivity intercept and comparison with specific refraction equations, J. Franklin Inst. 222 (1936) 563–592, https://doi.org/10.1016/S0016-0032(36)90986-9.