Prediction of Density, Dynamic Viscosity, and Surface Tension of Seven Ionic Liquids $[N_{222(n)}][Tf_2N]$ (n = 5,6,7,8,10,12,14)

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ABSTRACT: *In the present work, some thermophysical properties are correlated and predicted for seven Ionic Liquids (ILs) n-alkyl triethylammonium bis(trifluoromethylsulfonyl)imide ($[N_{222(n)}][Tf_2N]$). In this way, the Cubic Plus Association (CPA) Equation of State (EoS) singly, and in combination with the Free Volume Theory (FVT) and the modified Pelofsky models were employed to estimate the density, dynamic viscosity, and surface tension of the ILs, respectively. The properties of three of the ILs were correlated and the parameters of the models were optimized. Then, the achieved parameters were correlated as a unified-form function of carbon number in cationic alkyl chains of the ILs so that the model parameters could be predicted for the other four ILs. Indeed, three ILs with pentyl, octyl, and dodecyl alkyl chains were used in the correlation scenario, and the others were utilized in the predicting approach. According to the results, correlation, and prediction approaches present Absolute Average Deviations (AADs%) equal to 0.0207 & 1.1393 for density, 4.4478 & 12.8312 for dynamic viscosity, and 0.1632 & 1.3820 for surface tension, respectively. As can be concluded from the output, both correlative and predictive approaches demonstrate good accuracy. Therefore, the inter/extrapolation of the results could be performed for other ILs from this family.*

KEYWORDS: *CPA, FVT, Ionic liquids, Density, Viscosity, Surface tension.*

INTRODUCTION

The outstanding characteristics of Ionic Liquids (ILs) such as electrochemical/thermal stability, low combustibility, nonvolatility, and Tunability, nominate them for different small to large-scale applications from laboratory to industry [1]. Accordingly, they are welcomed in various fields, including separation (solid/liquid/vapor), catalysis, pharmaceuticals, additives, electrolytes, and many others. Therefore, measurement and/or calculation of their thermophysical properties (e.g., density, viscosity, and surface tension) play(s) a vital role in different uses.

Up to now, some experimental research has been performed to measure various physical properties of different ILs. Nevertheless, because of the innumerable variety of ILs and operational conditions, employing theoretical models could be a rescuing alternative. Therefore, many of these methods, such as using Equations of State (EoSs), have been proposed to model the thermophysical properties of ILs [2]. Indeed, thermodynamic properties could be calculated using EoSs.

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EoSs can provide thermodynamic derivative properties such as density accurately. Up to now, few EoS-based models have been successfully used to describe the thermophysical properties of fluids [3]. Among the applied models, associative EoSs such as CPA and Statistical Association Fluid Theory (SAFT) variants are the most promising EoSs that can be used to estimate the fluids' thermophysical properties. In this direction, *Llovell et al.* [4] combined the FVT model and soft-SAFT EoS to predict the viscosity of n-alkanes and their mixtures. Their approach presented an overall AAD% equal to 2.12.

Akbari and Alavianmehr [5], coupled the square-well model and the Perturbed-Hard-Trimmer-Chain (PHTC) EoS to obtain the surface tension of some alkanes and refrigerants in various temperatures. Their correlative approach presented Absolute Relative Deviation (ARD) equal to 2.46% for 251 data points.

The pseudolattice approach for the surface tension of IL Solutions was implemented by *Arjmand et al*. [6]. Their results present good applicability of the following approach to estimate the surface tension of the studied ILs.

Perturbed-Chain SAFT (PC-SAFT), Generalized SAFT (GSAFT)+cubic, and CPA EoSs were applied by *Polishuk* [7] to predict the thermodynamic properties of some ILs with [Tf_2N] anion. In another work [8], GSAFT+cubic EoS was implemented to predict some properties such as density, the velocity of sound, and isothermal and isotropic compressibility factors for some heavy alkanes/oils, and three imidazolium-based ILs.

Thermodynamic properties, including vapor pressure, liquid density, heat capacity, and sound speed, of gases related to CO_2 capture were calculated using SAFT and PC-SAFT EoSs in the work of *Diamantonis* and *Economou* [9].

Khoshnamvand and *Assareh* [10], applied the FVT accompanying PC-SAFT EoS to predict the viscosity of petroleum reservoirs. In their work, the viscosity of six real reservoirs was studied and AAD% = 9.7 was obtained. Their results accuracy shows at least 6% improvement compared to the standard industrial methods [10].

Two Artificial Intelligence (AI) based models, including Genetic Function Approximation (GFA), and Artificial Neural Network (ANN) were applied by *Golzar et al*. [11] to estimate the density, viscosity, and surface tension of five ILs [$N_{222(n)}$][Tf_2N] (n = 5,6,8,10,12). Their results will be used for comparison with the new output of this work.

Between different ILs, quaternary ammonium derivatives with [Tf_2N] anion present interesting performance in different applications [12]. Accordingly, the estimation of their physical properties is very important. Therefore, in the present work, the CPA EoS lonely and as innovative combinations with FVT and modified Pelofsky (mPelofsky) models employed for the first time to estimate the density, dynamic viscosity, and the surface tension of seven ILs n-alkyl-triethylammonium bis(trifluoromethyl-sulfonyl)imide ([$N_{222(n)}$][Tf_2N]) comprising of triethyl(pentyl)ammonium ([$N_{222(5)}$]), triethyl(hexyl) ammonium ([$N_{222(6)}$]), triethyl(heptyl)ammonium ([$N_{222(7)}$]), triethyl(octyl)ammonium ([$N_{222(8)}$]), triethyl(decyl)ammonium ([$N_{222(10)}$]), triethyl(dodecyl)ammonium ([$N_{222(12)}$]), triethyl(tetradecyl)ammonium ([$N_{222(14)}$]) cations and bis(trifluoromethyl-sulfonyl)imide ([Tf_2N]) anion.

THEORETICAL SECTION

Models

Cubic Plus Association (CPA) EoS

The classic CPA EoS has two main parts, including the SRK EoS and Wertheim's association term [13]. For a pure component, the CPA EoS can be simplified as below:

$$P = \frac{RT}{v-b} - \frac{a(T)}{v(v+b)} - \frac{RT(1-X^{A_i})}{v-0.475b} \quad (1)$$

X^{Ai} is the fraction of type A sites at molecule i that establishes no hydrogen bonds with the other association sites, and its value in the 2B association scheme can be calculated as:

$$X^{A_i} = \frac{-1+\sqrt{1+4\rho\Delta^{A_iB_j}}}{2\rho\Delta^{A_iB_j}} \quad (2)$$

Where Δ^{AiBj} represents association strength and is calculated through the below equation:

$$\Delta^{A_iB_j} = \frac{b\,\beta}{(1-0.475b\rho)}\left[exp\left(\frac{\varepsilon^{A_iB_j}}{RT}\right)-1\right] \quad (3)$$

In which ε^{AiBj} and β denote the association energy and volume, respectively.

$a(T)$ stands for the energy parameter that is calculated as:

$$a(T) = a_0\left[1+c\left(1-\sqrt{T_r}\right)\right]^2 \quad (4)$$

Where T_r is reduced temperature.

All the studied ILs were supposed to conform to the 2B association scheme wherein cations, and anions are the positive, and negative association sites, respectively.

Free Volume Theory (FVT)

According to the model [14], dynamic viscosity (η) of a dense fluid (e.g., liquids) could be determined utilizing the following relation:

$$\eta = 4.0785\times10^{-5}\frac{\sqrt{M_w T}}{v_c^{\frac{2}{3}}\Omega^*}(1-0.2756w)+ \rho L\frac{\left(E_0+\frac{PM_w}{\rho}\right)}{\sqrt{3RTM_w}}exp\left(B\left(\frac{E_0+\frac{PM_w}{\rho}}{2RT}\right)^{1.5}\right) \quad (5)$$

All the required details have been reported in [14].

As one can see, L, E_0, and B are the model optimizable parameters and are known as the free space formation parameter, the diffuse barrier energy of the molecule, and a dimensionless constant, respectively. In the following approach, the required density parameters in FVT are calculated by CPA using the obtained parameters in the previous section.

Modified Pelofsky model

Ghatee et al. [15] modified the proposed model by Pelofsky [16] for calculating the surface tension (γ) of the ILs. This model can be presented as:

$$ln\,\gamma = ln\,C + \frac{D}{\eta^{\phi}} \quad (6)$$

Where C and D are two constants related to the substances. Moreover, ϕ is known as the universal exponent, and its value is considered equal to 0.3 [15].

It should be mentioned that the dynamic viscosities in this part are estimated through FVT (and CPA EoS) using the obtained parameters in the previous sections. Indeed, a combinatorial approach has been employed.

Prediction function

In this work, a unified power-law function has been implemented for the first time to estimate all the predicted parameters of all the above-mentioned models.

$$PP = a'(n_c)^{b'} + c' \quad (7)$$

PP, and n_c stand for Predicting Parameters and carbon atom number in the alkyl chain of the cations of the ILs. Besides, a', b', and c' are fitting parameters, so they should be specified for each parameter. Indeed, this relation could be considered as a main novel objective of the work so that it can able one to predict the density, dynamic viscosity, and surface tension of the mentioned ILs, only by knowing the n_c parameter.

Methodology and used data sets

Experimental density, dynamic viscosity, and surface tension data for the ILs with 5, 6, 8, 10, and 12 carbon atoms in their cation's alkyl chain were extracted in the temperature range between 298 to 373 K [12]. In this way, sixteen data points for each property of each IL were provided. Moreover, for the ILs with 7 and 14 carbon atoms in their cationic alkyl chains, experimental data for all the properties were taken from [17] at temperatures from 293 to 363 K. Accordingly, eight data points for each property of the ILs were extracted. It should be remarked that because of the difference in the used methods, apparatuses, and material purities, the reported experimental data for a specific IL within a particular condition has some discrepancies in the two references. This discordance could absolutely affect the accuracy of the modeling by itself.

For all the investigated physical properties, ILs with pentyl, octyl, and dodecyl alkyl chains were studied in the correlation scenario so that the parameters of Eq. (7) were found in this way. After that, the other ILs with 6, 7, 10, and 14 carbon atoms in their alkyl chains were investigated in the predicting approach.

It is necessary to note here that, in the CORRELATION approach, the parameters of the models are optimized using different objective functions, while in the PREDICTION scenario, the correlated parameters are used without adjusting any new parameter. Thus, the higher AADs% for the predicted values could be expected.

RESULTS AND DISCUSSION

The Pure Component Physical Properties

To implement the mentioned models, some physical properties, including critical temperature (T_c), critical Pressure (P_c), critical volume (v_c), and acentric factor (w), were estimated using the "modified Lydersen-Joback-Reid (mKJR)" method by *Valderrama* and *Robles* [18]. Sufficient details about the used approach can be found in our previous works [19]. The obtained values have been reported in Table 1.

The CPA pure components parameters - Density calculation

Five adjustable parameters, including a_0, b, c_1, ε, and β, should be determined for each associating component using the CPA EoS [13]. To do this, vapor pressure and liquid density data are conventionally used. But, because ILs are

Table 1: Physical properties for the ILs.

Component	Mw	T_c (K)	P_c (bar)	ω	v_c (cm^3/mol)
$[N_{222(5)}][Tf_2N]$	452.47	1102.521	19.8048	0.5146	1183.92
$[N_{222(6)}][Tf_2N]$	466.5	1119.222	18.6876	0.5607	1241.03
$[N_{222(7)}][Tf_2N]$	480.53	1136.265	17.6839	0.6067	1298.14
$[N_{222(8)}][Tf_2N]$	494.55	1153.671	16.7773	0.6522	1355.25
$[N_{222(10)}][Tf_2N]$	522.61	1189.664	15.2069	0.7403	1469.47
$[N_{222(12)}][Tf_2N]$	550.66	1227.386	13.8947	0.8216	1583.69
$[N_{222(14)}][Tf_2N]$	578.72	1267.037	12.7837	0.8923	1697.91

Table 2: The CORRELATED CPA parameters for the ILs.

Component	a_0 (bar.L/mol^2)	b (L/mol)	c_1	ε^{AiBj} (bar.L/mol^2)	β	Ref.	N	AAD (ρ) %
$[N_{222(5)}][Tf_2N]$	11.3801	0.0003	0.0033	3129.6672	0.0017	[12]	16	0.0193
$[N_{222(8)}][Tf_2N]$	12.8479	0.0003	0.0025	3321.1091	0.0019	[12]	16	0.0266
$[N_{222(12)}][Tf_2N]$	14.7895	0.0004	0.0020	3618.4187	0.0020	[12]	16	0.0161
Average AAD%							48	0.0207

Table 3: The Eq. (7) parameters for density prediction and the PREDICTED CPA parameters.

Eq. (7) Coefficients	a´	b´	c´	a´	b´	c´	a´	b´	c´	a´	b´	c´	a´	b´	c´	Ref.	N	AAD(ρ) %
	0.51540	0.98190	8.87700	0.00019	0.31730	- 0.00002	0.00860	- 0.60420	0.00004	24.42000	1.35300	2914.000	0.00131	0.16760	0.00003			
Predicted Parameters / Comp.	a_0 (bar.L/mol^2)			b (L/mol)			c_1			ε (bar.L/mol^2)			β					
$[N_{222(6)}][Tf_2N]$	11.8707			0.0003			0.0029			3189.7937			0.0018			[12]	16	0.4013
$[N_{222(7)}][Tf_2N]$	12.3599			0.0003			0.0027			3253.7530			0.0019			[17]	8	1.1754
$[N_{222(10)}][Tf_2N]$	13.8206			0.0004			0.0022			3464.4852			0.0020			[12]	16	0.9400
$[N_{222(14)}][Tf_2N]$	15.7560			0.0004			0.0018			3781.8744			0.0021			[17]	8	2.9778
Average AAD%																	48	1.1393

almost non-volatile compounds, no vapor pressure data could be found in the literature. Therefore, experimental liquid density data are used to obtain the CPA parameters by minimizing the following objective function:

$$AAD(\rho)\% = \frac{100}{N}\sum_{i}^{N}\frac{\left|\rho_i^{exp} - \rho_i^{calc}\right|}{\rho_i^{exp}} \quad (8)$$

Where N is the total number of data points. The correlated pure parameters, and AAD% of the liquid density data, are presented in Table 2.

Using the obtained values in Table 2, the parameters of Eq. (7) were correlated. The calculated values have been presented in Table 3.

The presented results in Tables 2 and 3 demonstrate excellent correlatability and predictability of the used model. Accordingly, the obtained parameters could be utilized to calculate CPA parameters for other ILs from the $[N_{222(n)}][Tf_2N]$ family. Indeed, the density of pure ILs in this family could be estimated without using any experimental data.

It should be mentioned here that, as the experimental data of ILs $[N_{222(7)}][Tf_2N]$ and $[N_{222(7)}][Tf_2N]$ have been taken from different references, some discrepancies in the results are not far from expectation. This is because of the fact the achieved parameters of Eq. (7), have been estimated using experimental data from Reference [12] while were applied to predict viscosity values from reference [17]. In other words, the experimental data of reference [17] were only employed in the prediction scenario. Therefore, the obtained values could be interpreted as the excellent predictability of the CPA EoS.

Fig. 1 presents Experimental vs. Calculated densities in different temperatures using SRK-CPA EoS.

Dynamic viscosity (η) calculation

The dynamic viscosity (η) of the ILs was calculated by

Table 4: The CORRELATED FVT parameters for the ILs.

Component	L × 10^{10} (m)	E_0 (kJ/mol)	B	Ref.	N	AAD (η) %
$[N_{222(5)}][Tf_2N]$	1.2762	20279.9817	0.2806	[12]	16	4.2672
$[N_{222(8)}][Tf_2N]$	0.8462	28012.9256	0.2162	[12]	16	4.1084
$[N_{222(12)}][Tf_2N]$	0.7639	31768.3222	0.1794	[12]	16	4.9677
Average AAD%					48	4.4478

Table 5: The parameters of Eq. (7) for viscosity prediction and the PREDICTED FVT parameters.

Eq. (7) Coefficients	a'	b'	c'	a'	b'	c'	a'	b'	c'	Ref.	N	*AAD (η) %*
	124.6000	- 3.3810	0.7359	- 1.378×10^5	- 1.3050	3.715×10^4	0.8195	- 0.9408	0.1003			
Predicted Parameters / Comp.	$L \times 10^{10}$ (m)			E_0 (kJ/mol)			B					
$[N_{222(6)}][Tf_2N]$	1.0274			23852.7499			0.2522			[12]	16	8.3203
$[N_{222(7)}][Tf_2N]$	0.9090			26275.8261			0.2317			[17]	16	11.4751
$[N_{222(10)}][Tf_2N]$	0.7877			30322.6964			0.1942			[12]	16	4.5912
$[N_{222(14)}][Tf_2N]$	0.7525			32748.9923			0.1687			[17]	16	26.9381
Average AAD%											64	12.8312

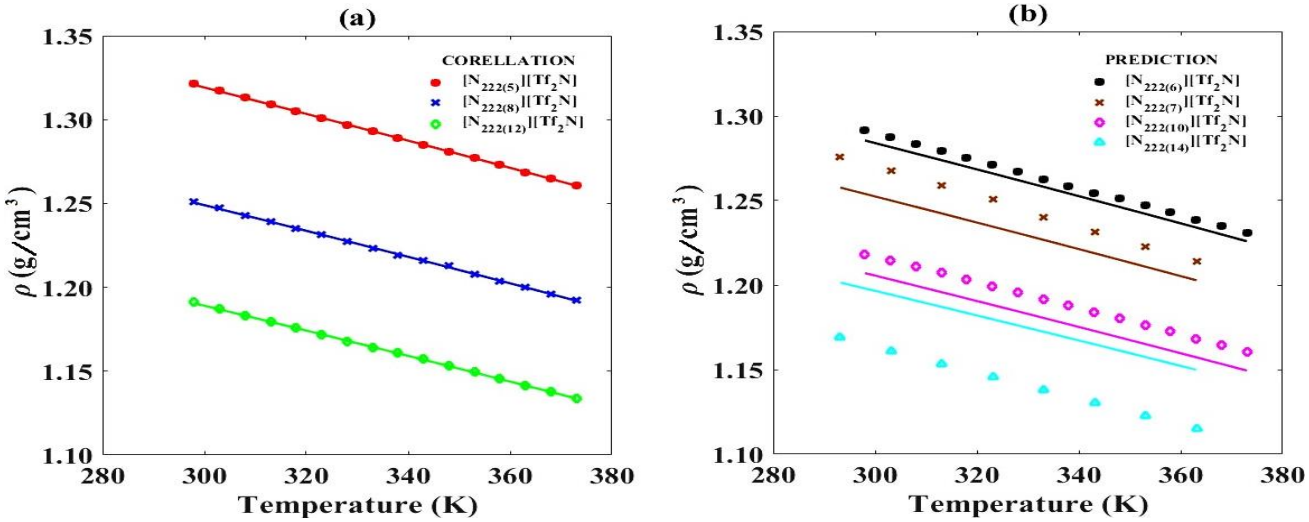

Fig. 1: Experimental (nodes) vs. Calculated (Lines) densities in different temperatures using the SRK-CPA EoS in (a): CORRELATION and (b): PREDICTION scenarios.

applying the FVT model. To do this, density values are required. Therefore, the obtained densities in the previous section are used.

To achieve the model parameters, dynamic viscosity data were utilized to minimize the following objective function:

$$AAD\ (\eta)\% = \frac{100}{N}\sum_{i}^{N}\frac{\left|\eta_i^{exp} - \eta_i^{calc}\right|}{\eta_i^{exp}} \qquad (9)$$

The obtained FVT parameters in the correlation scenario have been presented in Table 4.

The reported results in Table 4 show a good correlation of the used models. Using the obtained values in Table 4, the parameters of Eq. (7) were correlated. The calculated values have been presented in Table 5.

Table 5 illustrates the good predictability of the used models. It should be noted that in the viscosity prediction scenario, the required density values are also predicted. Indeed, no experimental data is used in this approach, neither for density nor viscosity calculation. Therefore, the outputs present pure prediction results.

Table 6: Comparison between calculated viscosities using different models.

	ILs / Model	$[N_{222(5)}][Tf_2N]$	$[N_{222(6)}][Tf_2N]$	$[N_{222(8)}][Tf_2N]$	$[N_{222(10)}][Tf_2N]$	$[N_{222(12)}][Tf_2N]$	Overall AAD%	Ref.
AAD (η) %	*Arrhenius*	9.80	9.20	9.00	10.60	9.80	9.68	[12]
	Litovitz	2.20	3.20	0.98	8.80	1.90	3.42	[12]
	CPA+FVT	4.27	8.32	4.11	4.59	4.97	5.25	This Work

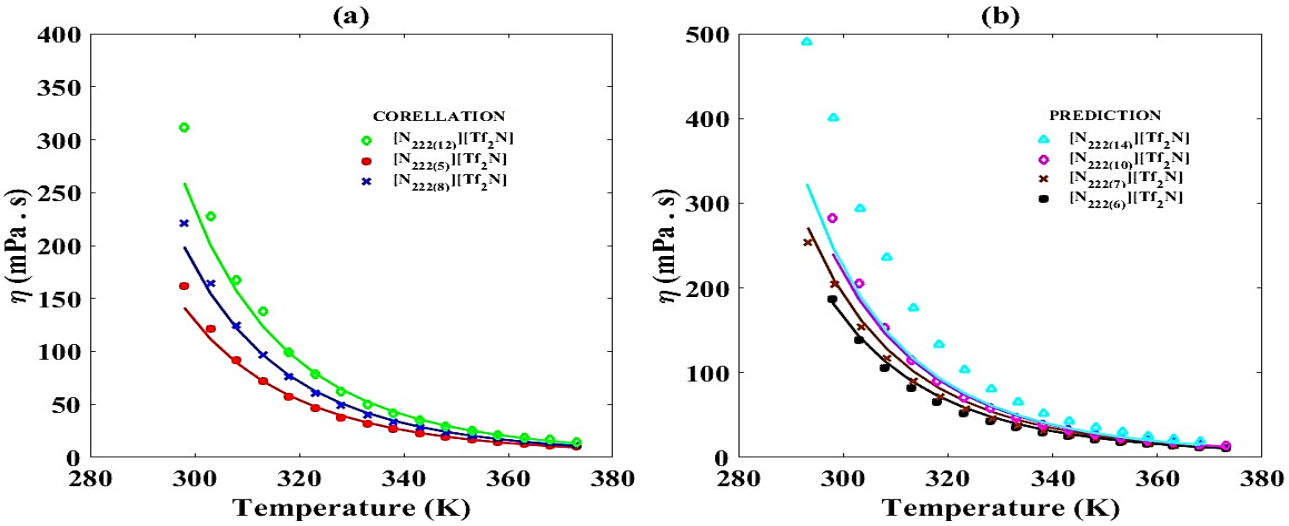

Fig. 2: Experimental (nodes) vs. Calculated (Lines) dynamic viscosities in different temperatures using the FVT+ CPA model in (a): CORRELATION and (b): PREDICTION scenarios.

Fig. 2 presents Experimental and Calculated viscosities in different temperatures using the FVT+ CPA model for both CORRELATION and PREDICTION scenarios.

As it can be seen, maximum AADs% are calculated for ILs $[N_{222(7)}][Tf_2N]$ and $[N_{222(7)}][Tf_2N]$. This is because the used experimental data for these two ILs were obtained from a different resource. Accordingly, good predictability of the applied models can be concluded.

The obtained AADs% results for viscosity estimation using two well-known models Arrhenius and Litovitz, with those of CPA+FVT have been compared in Table 6. It should be emphasized that the results of the Arrhenius and Litovitz models are correlated directly using experimental viscosity data while in the present approach (CPA+FVT), the required density was calculated using CPA, and then viscosities were obtained by FVT. Besides, results for hexyl and decyl ILs are purely predictions.

As anybody can conclude, the new results present better accuracies, with higher prediction capability.

Surface tension (γ) calculation

Using the modified Pelofsky (mPelofsky) model [15] to calculate surface tension needs dynamic viscosity values. Therefore, the calculated viscosities in the last section are used. For the sake of the lack of experimental surface tension data for ILs with 7 and 14 carbon atoms in their alkyl chain, these ILs are not investigated in this section. The experimental data for the other ILs were obtained from [12].

To optimize the parameters of the model, the following objective function should be minimized:

$$AAD\ (\gamma)\% = \frac{100}{N}\sum_{i}^{N}\frac{\left|\gamma_i^{exp} - \gamma_i^{calc}\right|}{\gamma_i^{exp}} \qquad (10)$$

The obtained mPelofsky model parameters in the correlation scenario are reported in Table 7.

The correlation results show excellent accuracy for calculating the surface tension of the ILs. Using these values, the parameters of Eq. (7) were computed. The calculated values have been presented in Table 8.

The average *AAD%* equal to 1.382 was obtained for predicted surface tensions. Thus, good predictability of the used models is seen. It should be noted that, in the prediction scenario, the predicted viscosity values are utilized. Indeed, no experimental data is needed.

Fig. 3 illustrates the experimental and calculated surface tensions (γ) in different temperatures using the

Table 7. The CORRELATED mPelofsky model parameters for the ILs.

Component	ln(C (mJ/m^2))	D	Ref.	N	AAD (γ) %
$[N_{222(5)}][Tf_2N]$	3.7027	- 0.5635	[12]	16	0.0714
$[N_{222(8)}][Tf_2N]$	3.6410	- 0.7164	[12]	16	0.1874
$[N_{222(12)}][Tf_2N]$	3.6164	- 0.8579	[12]	16	0.2307
Average AAD%				48	0.1632

Table 8. The parameters of Eq. (7) for surface tension prediction and the PREDICTED mPelofsky model parameters.

Eq. (7) Coefficients	a'	b'	c'	a'	b'	c'	Ref.	N	AAD (γ) %
	1.8330	- 1.7470	3.5930	- 1.5060	0.1606	1.3870			
Predicted Parameters / Component	ln(*C* (mJ/m^2))			*D*					
$[N_{222(6)}][Tf_2N]$	3.6731			- 0.6212			[12]	16	2.3875
$[N_{222(10)}][Tf_2N]$	3.6169			- 0.8576			[12]	16	0.3764
Average AAD%								64	1.3820

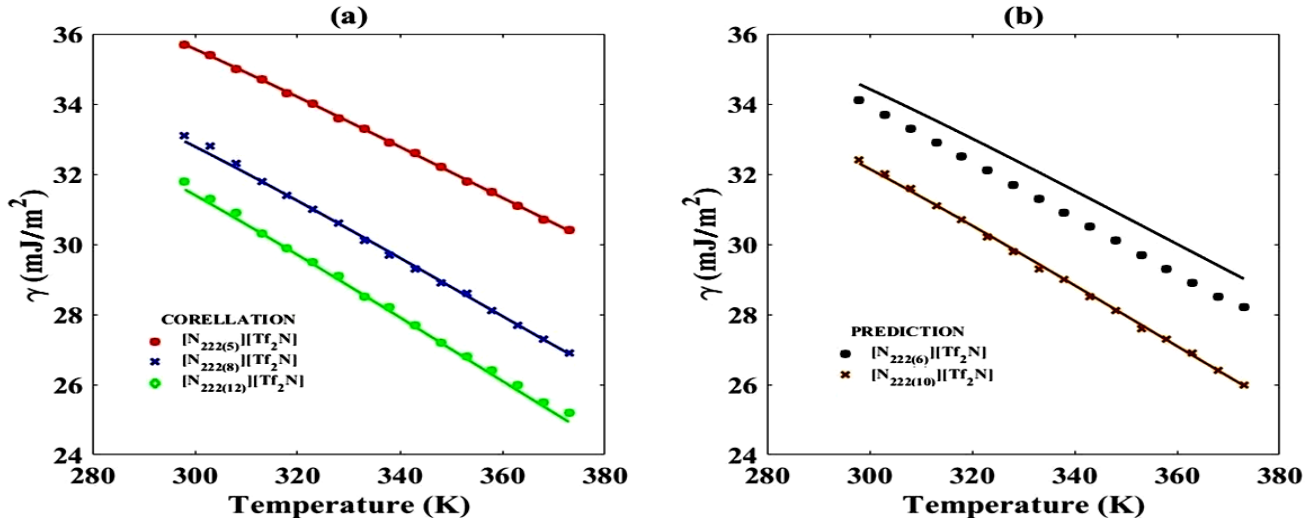

Fig. 3: Experimental (nodes) vs. Calculated (Lines) surface tensions (γ) in different temperatures using the mPelofsky+ FVT+ CPA models in the CORRELATION and PREDICTION scenarios.

Table 9: Comparison between overall AADs% for calculated densities using different models.

	Models / Approach	Density			Viscosity			Surface Tension		
		GFA	ANN	CPA	GFA	ANN	CPA+FVT	GFA	ANN	CPA+FVT+mPelofsky
Overall AAD (ρ) %	CORRELATION	0.69	0.04	0.02	67.72	4.20	4.45	0.49	0.34	0.16
	PREDICTION	0.81	0.04	0.67	139.51	6.60	6.46	0.45	0.38	1.38
	Ref.	[11]	[11]	This Work	[11]	[11]	This Work	[11]	[11]	This Work

mPelofsky+ FVT+ CPA models in the CORRELATION and PREDICTION scenarios.

Comparison of the results with AI-based models

The obtained overall AADs% for density, viscosity, and surface tension calculations were compared with those estimated using accurate GFA and ANN models in Table 9. It should be mentioned that the used data in the different models are not the same, but only a rough comparison is considered. As one can see, the correlatability and predictability of the used approaches are apparent.

CONCLUSIONS

This work was dedicated to correlating and predicting the density, dynamic viscosity, and surface tension of seven ILs of the ($[N_{222(n)}][Tf_2N]$) family with 5, 6, 7, 8, 10,

12, and 14 carbon atoms in their cation alkyl chains. Three of them, including pentyl, octyl, and dodecyl alkyl chain ILs, were studied in the correlation approach, while the others were investigated in the prediction procedure.

CPA EoS was implemented to estimate liquid density with AADs% equal to 0.0207 & 1.1393 for correlation and prediction scenarios, respectively. Also, FVT+ CPA was employed to obtain dynamic viscosities while mPelofsky+ FVT+ CPA was applied to calculate surface tension. Overall AADs% were calculated 4.4478 & 12.8312 for viscosity and 0.1632 & 1.3820 for surface tension correlation & prediction approaches, respectively.

It should be added here that the adjusted parameters were optimized based on the experimental data of the ILs with pentyl, octyl, and dodecyl alkyl chains from a specific data set, and then the same parameters were employed to predict the properties of the ILs with heptyl and tetradecyl alkyl chains from another dataset.

Finally, a rough comparison between the obtained results and those obtained using AI-based models was performed. According to the outputs, the used models present good correlatability, and predictability so that the properties of other ILs from this family could be estimated in different conditions with reasonable accuracies.

Nomenclature

Absolute Average Deviation	AAD
Absolute Relative Deviation	ARD
Temperature function of the SRK EoS	a(T)
Fitting parameter of Eq. (7)	a
Fitting parameter of Eq. (4)	a_0
A dimensionless constant of the FVT model	B
Excluded volume (Constant of SRK EoS)	b
Fitting parameter of Eq. (7)	b
Constant of SRK EoS	c_1
Fitting parameter of Eq. (7)	c
mPelofsky model parameters	C, D
Molecule diffuse barrier energy (kJ/mol)	E_0
Boltzmann's constant (1.38066×10^{-23} J/K)	k
Free space formation parameter (m)	L
Molecular weight	M_w
Number of data points	N
Total pressure	P
Predicted parameter	PP
Critical pressure	P_C
Universal gas constant (8.31415 J/mol/K)	R
Absolute temperature (K)	T
Critical temperature (K)	T_C
Reduced temperature	T_r
Molar volume	v
Critical volume	v_C
Acentric factor	w
Fraction of A-type unbounded sites on molecule i	X^{Ai}
Association strength	Δ^{AiBj}
Association volume	β
Surface tension (mJ/m^2)	γ
Association energy	ε^{AiBj}
Dynamic viscosity (mPa.S)	η
Density	ρ
An empirical relation in Eq. (5)	**Ω***
Calculated	Cal.
Experimental	Exp.

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