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Measurement and prediction of the physical properties of an aqueous sodium salt of L-phenylalanine

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Abstract: Physical properties, such as density, refractive index and viscosity, of an aqueous sodium salt of (S)-2-amino-3-phenylpropionic acid (L-phenylalanine, Na-Phe) were investigated in this work. These properties were measured over a temperature range of 298.15–343.15 K at atmospheric pressure. The mass fractions (w) of Na-Phe were 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.35 and 0.40. The analysis of the experimental data showed that the values of density, refractive index and viscosity decreased with increasing temperature at any constant concentration of Na-Phe. However, these values increased with increasing concentration at any constant temperature. The density values were used to estimate the thermal expansion coefficient. The thermal expansion coefficient increased slightly with increasing temperature and concentration. The density and refractive index data were correlated using a modified Graber equation, while, the viscosity data were correlated using a modified Vogel–Tamman–Fulcher (VTF) equation. In all the cases, quantitative analyses of the influence of temperature and concentration were performed.

Keywords: density; refractive index; viscosity; thermal expansion coefficient; ANOVA.

INTRODUCTION

The increasing emissions of greenhouse gases (GHGs), mainly due to the advancement of technology and rapid industrialization, significantly contribute towards global warming. Carbon dioxide is a major greenhouse gas responsible for global warming.[1,2] According to recent guidelines and mitigation policies of the International Energy Agency (IEA), the world-wide energy-related CO_2 emissions may reach almost 45 Gt by the year 2035, which could further increase the global temperature to 5.6 °C.[3] In this regard, it is very important to focus on research for the development of cost-effective CO_2 capture technologies. Dif-

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ferent methods have been used to remove CO_2 from flue gases emitting from power plants and other industries. Among these, chemical absorption using alkanolamines is currently the most favorable method for CO_2 capture.[4–8] The most commonly used alkanolamines for CO_2 absorption process are 2-aminoethan-1-ol (monoethanolamine, MEA), 2,2′-iminodiethanol (diethanolamine, DEA), 2,2′-(methylazanenedyl)di(ethan-1-ol) (*N*-methyldiethanolamine, MDEA) and 2-amino-2-methyl-1-propanol (AMP).[9,10] Initially, the use of these solvents was favored due to several advantages, such as the presence of alcohol groups, which significantly decrease the vapor pressure of the amine, and aids in the decontamination of the gases being treated.[11,12] However, various drawbacks of these solvents have been highlighted and reported by many researchers after thorough investigations.[13,14] These drawbacks include short lifetime due to thermal and oxidative degradation, and excessive corrosion of equipment, which results in the reduction of equipment life, production losses, and other additional costs for the restoration of the corroded system. Additionally, high regeneration energy, solvent loss due to high volatility, and toxic nature of these solvents restrict their use for CO_2 capture processes.[15]

Amino acid salts have been identified as potential solvents for CO_2 capture due to their significant advantages over amines.[16–19] Amino acid salts behave in the same way as amines in the CO_2 removal process owing to the similar functional group, but have different positive characteristics as CO_2 removal agents. The main advantages of amino acid salts include better resistance towards oxidative and thermal degradation, negligible volatility due to the ionic structure, which prevents vapor loss at high temperatures.[20–25] Additionally, amino acids have the ability to regenerate, are environmentally friendly, and easily available on the commercial scale.[26,27] These benefits of amino acid salts make it interesting and important to perform thorough investigation on these solvents for CO_2 capture processes. Studies involving various amino acids with different salts, such as sodium, potassium, and lithium, have already been conducted, which showed that these are the promising solvent systems for the CO_2 capture process.[1,23,28–31]

Physical properties are important for a detailed molecular interpretation of a given solvent at different solute concentrations and temperatures, and simultaneously determine the effects of temperature and concentration on such properties.[32–37] These findings could be useful in the suggestion of new amino acid salt-based solutions for CO_2 absorption.[38] In order to determine the effect of temperature on the change in volume of the studied aqueous solutions, the coefficient of thermal expansion was estimated. To the best of our knowledge, no data for the physical properties of aqueous solution of the sodium salt of L-phenylalanine (Na-Phe) are available in the open literature. Therefore, in this study, the physical properties, *i.e.*, density, refractive index, and viscosity, of aqueous

Na-Phe solutions were determined studied and reported. Additionally, all physical properties were correlated using empirical correlations, such as function of temperature and concentration along with detailed statistical evaluation of empirical correlations. The correlations used in this study are solely based on the analysis of deviation, and have been used by many authors.[39–41]

EXPERIMENTAL

Samples preparation

All the chemicals used in this study were purchased from Merck (Malaysia). The specifications of the chemicals used are given in Table S-I of the Supplementary material to this paper. The aqueous solutions of the sodium salt of L-phenylalanine (Na-Phe) were prepared by neutralizing the amino acid with an equimolar quantity of sodium hydroxide dissolved in double distilled water. The same procedure was used in literature.[15,29,42] Weight measurements were realized using a digital electronic balance (Sartorius BSA224S-CW), which has an accuracy of $\pm 10^{-4}$ g. Different mass fractions (w) of aqueous Na-Phe were 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.35 and 0.40. All physical properties were measured in the temperature range 298.15–343.15 K. The selected concentration and temperature range of the solvent were based on the commercial applicability and suitability of the solvent for the CO_2 removal process.[42] The estimated uncertainty in the experimental concentration was $\pm 10^{-3}$.

Details about calibration of the apparatus as well as density, refractive index and viscosity measurements are described in Supplementary material.

RESULTS AND DISCUSSION

Effect of temperature and concentration on density

The experimental density data for the aqueous solutions of the sodium salt of L-phenylalanine (Na-Phe) were measured over a mass fraction range of 0.05 to 0.40 and temperature ranging from 298.15 to 343.15 K. The measured density data are presented in Table S-III of the Supplementary material, and Fig. 1 shows the effect of temperature and concentration on the density of aqueous Na-Phe solutions. It is apparent that the density increased as the concentration of Na-Phe in the solution increased isothermally, thus showing the effect of concentration. As mentioned in the introduction, both amino acid salts and amines have an amino group ($-NH_2$) in their structure.

Therefore, similar to amines, the amino acid salt (Na-Phe) molecules also form hydrogen bonds with each other as well as with water.[43,44] Moreover, van der Waals dispersion forces and dipole–dipole interactions (also known as intermolecular forces) exist between Na-Phe molecules.[44] Thus, due to increased intermolecular interactions and H-bonding between Na-Phe and water molecules at higher concentrations, the density values increase.[15,42,45] At a uniform temperature (298.15 K) and at the lowest mass fraction (0.05), the value of density of the aqueous solution of Na-Phe was 1.01297 g cm^{-3}. With an average linear increase of 1.53 % (or 0.016277 g cm^{-3}), the maximum value of density was found to be 1.12691 g cm^{-3} at a mass fraction of 0.40. Additionally, the density data showed a decreasing trend with increasing temperature of the aqueous Na-Phe solution. This may be due to extensive spaces between the molecules at higher temperatures, which results in expansion of the solution volume and thus, reduced density.[46] The maximum density of an aqueous Na-Phe solution at the highest temperature (343.15 K) was 1.09800 g cm^{-3}. With a linear decrement in density values with increasing temperature, the minimum density of an aqueous Na-Phe was 0.99247 g cm^{-3}. The same behavior was reported in previous works on density measurements, which is also usually common for solutions of amino acid salts.[15,32,42,47]

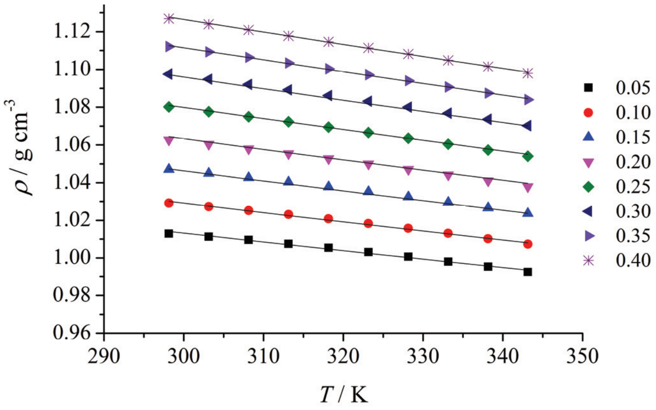

Fig. 1. Effect of temperature on the density of aqueous solutions of Na–Phe for various mass fractions. Symbols refer to experimental data points and lines refer to correlated data points.

Effect of temperature and concentration on the refractive index

The refractive index of aqueous Na-Phe solutions were measured over a mass fraction range of 0.05 to 0.40 and temperature ranging from 298.15 to 343.15 K, with a 5 K interval. The measured data are listed in Table S-IV of the Supplementary material, and the effects of temperature and concentration on the refractive index are shown in Fig. 2. It is evident from Fig. 2 that with increasing concentration of aqueous Na-Phe solution at any given temperature, the refractive index increases. The refractive index increases due to the higher availability of molecules resulting in the possibility of stray light to hit more molecules.[15,39] At a uniform temperature (298.15 K) and at the lowest mass fraction (0.05), the value of refractive index of the aqueous Na-Phe solution was n_D 1.34321. With an average linear increase of 0.010531, the refractive index increased to the maximum value of n_D 1.41603 at a mass fraction of 0.40.

Additionally, the obtained results indicated a decreasing trend in the refractive index values with increasing temperature of the aqueous Na-Phe solutions at any given concentration. The decreasing effect of the refractive index with increasing temperature is due to increased scattering in the sodium L-phenylalanine molecules, causing the stray light to hit fewer molecules that resulted in a reduced refractive index.[41] The maximum refractive index of aqueous Na-Phe at the highest temperature (343.15 K) was n_D 1.40472. While, with a monotonous decrease in the refractive index with increasing temperature, the lowest refractive index was n_D 1.33434. Similar observations were reported previously.[33,47,48]

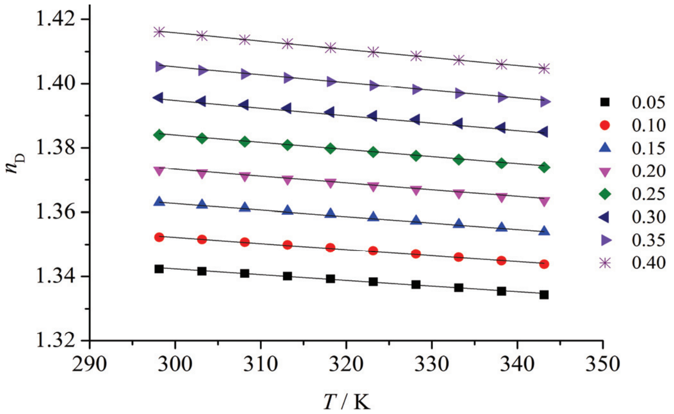

Fig. 2. Effect of temperature on the refractive index of aqueous Na-Phe solutions for various mass fractions. The symbols refer to the experimental data points and the lines refer to the correlated data points.

Effect of temperature and concentration on viscosity

The viscosity of aqueous the Na-Phe solutions were measured over a mass fraction range of 0.05 to 0.40 and temperature ranging from 298.15 to 343.15 K, with a 5 K interval. The measured viscosity data are presented in Table S-V of the Supplementary material, and the effects of temperature and concentration on the viscosity are shown in Fig. 3. It could be seen from Fig. 3 that there is a non--linear increase in viscosity with increasing concentration of the aqueous Na-Phe solutions. Since more molecules were available in the solution, the chances of collisions and formation of bonds between the molecules increased; however occasionally collisions might also provide energy to break bonds.[49] At a constant temperature of 298.15 K and at the lowest mass fraction of 0.05, the value of viscosity of aqueous Na-Phe solution was 0.991 mPa s. With an average non--linear increase of 0.752 mPa s, the viscosity increased to a maximum value of 6.254 mPa s at a mass fraction of 0.40. Additionally, the results demonstrated an exponential decrease in viscosity of aqueous Na-Phe solution with increasing solution temperature at any given concentration.

A probable clarification for this type of behavior is that, as the temperature rises, the speed of the interacting molecules inside solution increases, which in turn reduces the interaction between the molecules.[39] Moreover, the intermolecular force between the solvent molecules is reduced at high temperature, and so is the viscosity.[39] The maximum viscosity of the aqueous Na-Phe solutions at the highest temperature of 343.15 K was 1.729 mPa s. While, with an exponential decrease in viscosity values as the temperature rises, the lowest value of viscosity was 0.446 mPa s. The consistency in the difference of the viscosity of the solutions follows the trend observed in the published literature for similar types of aqueous systems.[15,41,42,47]

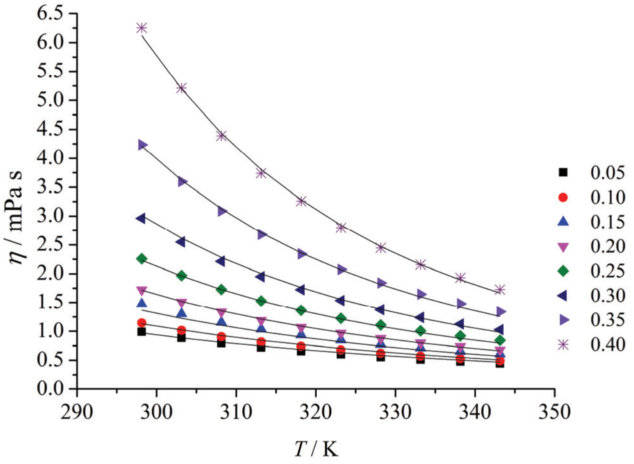

Fig. 3. Effect of temperature on the viscosity of aqueous Na-Phe solutions for various mass fractions. Symbols refer to the experimental data points and the lines refer to correlated data points.

Correlations for physical properties

For the purpose of future applications in CO_2 absorption processes, all physical properties were correlated as a function of both temperature and concentration. Many researchers have used correlations involving single variable (temperature or concentration) to represent physical property data.[33,46,47] The limitation of single variable correlation is that there are numerous equations to represent the data of corresponding physical property. Therefore, it is recommended to represent the data with a single equation comprising both variables, such as, temperature and concentration. Therefore, in the present study, a modified form of the equation earlier used by Graber *et al.*[50] was utilized to correlate the experimental density and refractive index data. This modified form of the equation was previously used by various researchers.[39,41,51] The following modified equation was used:

$$X = w\exp(A_1 + A_2T^{0.5} + A_3w^{0.5}) + A_4 + A_5T^{0.5} + A_6w^{0.5} \tag{1}$$

where X can be either density or refractive index, w is the mass fraction of the sodium salt of L-phenylalanine (Na-Phe), T is the temperature and A_i (i =

= 1,2,…,6) are empirical parameters determined by fitting the experimental values of density and refractive index to Eq. (1). The parameters were optimized by minimizing the objective function, represented by the *ARD* value:[46]

$$ARD = \frac{100}{n}\sum_{i=1}^{i=n}\left|\frac{|x_{\text{exp}} - x_{\text{corr}}|}{x_{\text{exp}}}\right| \tag{2}$$

where x_{exp}, x_{corr} and n represent the experimental data, the correlated data and the number of data points, respectively. The correlated density and refractive index data from Eq. (1) are shown graphically in Figs. 1 and 2 as lines. The optimized values of the empirical parameters, A_i, of Eq. (1) are presented in Table I.

To correlate the experimental viscosity data for aqueous Na-Phe solutions, a modified form of the Vogel–Tamman–Fulcher (VTF) equation was used.[52,53] The general form of the VTF asymptotic exponential function can be represented as:

$$\ln\ \eta = \ln y_{\text{c}} - \frac{E}{R(T - T_{\text{c}})} \tag{3}$$

where η is the experimental viscosity, y_{c} is the pre-exponential function, T and T_{c} are the experimental and critical-limit temperature, respectively, E is the activation energy and R is the universal gas constant. At $T_{\text{c}} = 0$, Eq. (3) is transformed into an Arrhenius-type equation, represented as:

$$\ln\eta = \ln y_{\text{c}} + \frac{B}{T} \tag{4}$$

where B is the ratio of the activation energy and the universal gas constant.

TABLE I. Fitting parameters of Eq. (1) for density and refractive index

Measurement	Parameter		No. of data points
	i	A_i	
ρ / g cm^{-3}	1	0.504800	80
	2	–0.037080	
	3	–0.701400	
	4	1.277000	
	5	–0.015070	
	6	–0.179000	
n_{D}	1	–0.626900	80
	2	–0.029140	
	3	–0.270100	
	4	1.441000	
	5	–0.005934	
	6	–0.049260	

To acquire a better fit of the experimental and correlated viscosity data, Eq. (4), was further modified by incorporating a second-order term and representing

B in the form of the mass fraction of the aqueous Na-Phe solutions. The second-order term (B_2/T^2) was added based on the distinctive behavior of ionic liquids, as previously studied by Hsieh *et al.*,[54] which could also be employed for aqueous amino acid salt solutions.[39,41] Now, the Arrhenius-type equation presented in Eq. (4) can be re-written as:

$$\eta = \exp\left[B_0 + \frac{B_1}{(T)} + \frac{B_2}{(T^2)}\right] \tag{5}$$

where B_j represents the empirical parameters that are dependent on the mass fraction (w) of the aqueous Na–Phe solutions and are represented by Eq. (6):

$$B_j = b_{j,0} + b_{j,1}w + b_{j,2}w^2 \tag{6}$$

where $b_{j,0}$, $b_{j,1}$ and $b_{j,2}$ are empirical parameters calculated by fitting the experimental viscosity data to Eqs. (5) and (6), which were similarly optimized by minimizing the objective function defined by Eq. (2). The correlated viscosity data from Eq. (5) is shown graphically in Fig. 3 as lines. The values of the optimized parameters $b_{j,0}$, $b_{j,1}$ and $b_{\mathrm{j},2}$ are listed in Table II.

TABLE II. Fitting parameters of Eq. (5) for viscosity

Measurement	Parameter				No. of data points
	i	$b_{j,0}$	$b_{j,1}$	$b_{j,2}$	
η / mPa s	1	–5.178	–8.056	1.804	80
	2	1500	2987	1647	
	3	26.43	161.5	26.44	

An additional property, *i.e.*, the coefficient of thermal expansion (α_{P}), was calculated using the density data. The coefficient of thermal expansion was calculated by correlating the density data as a linear function of temperature at constant pressure using Eq. (7):[15,55]

$$\alpha_{\mathrm{P}} = -\frac{1}{\rho}\left(\frac{\partial\rho}{\partial T}\right)_P = -\frac{C_1}{C_0 + C_1 T} \tag{7}$$

where ρ is the density, T is temperature, $(\partial\rho/\partial T)_{\mathrm{P}}$ is the slope of density data calculated using linear plot of density data as a function of temperature and C_0 and C_1 are the fitting parameters. A similar method of determining coefficient of thermal expansion could be found in the literature.[15,42,56,57] The values of coefficient of thermal expansion at different temperatures and concentrations are listed in Table III, whereas the values of fitting parameters C_0 and C_1 are presented in Table S-VI of the Supplementary material. It is apparent from Table III that there is a slight increase in the values of coefficient of thermal expansion with respect to temperature and concentration. Thus, it could be concluded that the present solvent would not expand substantially with increasing temperature of the aqueous system. The same trend was previously reported for similar types of systems by many researchers.[15,55,58]

TABLE III. Coefficient of thermal expansion (α_P / 10^{-4} K^{-1}) of aqueous sodium salt L-phenylalanine solutions

T / K	w							
	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40
298.15	4.52	4.73	4.98	5.20	5.38	5.53	5.63	5.71
303.15	4.53	4.74	4.99	5.21	5.40	5.55	5.64	5.72
308.15	4.54	4.75	5.00	5.22	5.41	5.56	5.66	5.74
313.15	4.55	4.76	5.01	5.23	5.42	5.58	5.67	5.75
318.15	4.55	4.77	5.02	5.25	5.44	5.59	5.69	5.77
323.15	4.56	4.78	5.04	5.26	5.45	5.61	5.70	5.79
328.15	4.58	4.79	5.05	5.27	5.47	5.62	5.72	5.80
333.15	4.59	4.81	5.06	5.29	5.48	5.64	5.74	5.82
338.15	4.60	4.82	5.08	5.30	5.50	5.66	5.76	5.84
343.15	4.61	4.83	5.09	5.32	5.52	5.68	5.77	5.86

Statistical analysis of the correlations

A detailed analysis of statistical parameters (*i.e.*, least square correlation coefficient (R^2), root mean-square error (*RMSE*), standard deviation (*SD*), average absolute deviation (*AAD*) and average relative deviation (*ARD*) was performed and the results are presented in Table IV. A detailed statistical analysis based on various statistical parameters is crucial for a thorough evaluation of the correlations used in this study. The equations used to calculate the statistical parameters are given as follows:

$$R^2 = \frac{\sum_{i=1}^{i=n}\left(x_{\mathrm{exp}} - x'_{\mathrm{corr}}\right)^2 - \sum_{i=1}^{i=n}\left(x_{\mathrm{exp}} - x_{\mathrm{corr}}\right)^2}{\sum_{i=1}^{i=n}\left(x_{\mathrm{exp}} - x'_{\mathrm{corr}}\right)^2} \tag{8}$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{i=n}\left(x_{\mathrm{corr}} - x_{\mathrm{exp}}\right)^2}{n}} \tag{9}$$

$$SD = \sqrt{\frac{\sum_{i=1}^{i=n}\left(x_{\mathrm{exp}} - x_{\mathrm{corr}}\right)^2}{n-1}} \tag{10}$$

$$AAD = \frac{\sum_{i=1}^{i=n} \left| x_{\exp} - x_{\mathrm{corr}} \right|}{n} \tag{11}$$

where $x_{\exp}$, x_{corr}, x'_{corr}, and n are the experimental data, correlated data, mean correlated data and the number of data points, respectively.

TABLE IV. Evaluation of statistical parameters for density, refractive index and viscosity

Parameter	Density	Refractive index	Viscosity
R^2	0.9996	0.9998	0.9988
RMSE	0.0007	0.0003	0.0416
SD	0.0007	0.0003	0.0394
ARD / %	0.0539	0.0194	2.6191
AAD / %	0.0006	0.0003	0.0313

For the graphical representation of the statistical analysis, relative error analysis and cross plots were sketched as shown in Figs. S-1 and S-2 of the Supplementary material. The relative error value of the correlated physical property of aqueous amino acid salt solutions is characterized as the percentage difference between the experimental and correlated values, which is plotted against the experimental values in Fig. S-1 (a–c).[59] Whereas, the cross plots could be defined as the graphical representation of experimental and calculated/correlated values against the line $y = x$.

It is apparent from Fig. S-1 (a–c) that both the number of data points and distribution of the relative error values on both sides of the zero line are very similar, which show that no systematic error exists in the applied correlations. Similarly, from Fig. S-2 (a–c), it could be observed that the experimental and correlated data sets fall mainly on the line $y = x$, which shows good agreement between both data. Thus, the applied correlations could be used satisfactorily to predict the data of physical properties for the present aqueous system within the studied experimental conditions of temperatures and concentrations.

Analysis of variance (ANOVA)

The ANOVA technique was applied to define the importance and impact of every factor included in the investigation of the physical properties of aqueous Na-Phe solutions. This technique is crucial for a better understanding of the statistical analysis of the experimental data and was previously used by various researchers.[42,60,61] The effect of concentration and temperature on different physical properties was examined through a two-factor without replication strategy in ANOVA. During the analysis, the default value of the significance level indicated by α was 0.05.[61] The variance analyses for density, refractive index, viscosity, and coefficient of thermal expansion of aqueous Na-Phe solutions are presented in Tables V–VIII, respectively. The term *df* represents the degree of freedom (calculated as the number of total levels –1), *SS* represents the sum of squares, and *MS* represents the mean squares (calculated as the ratio of *SS*/*df*). The *F*-values in ANOVA are a tool to aid in the determination of whether or not the variance between the means of two populations is significantly different. The *F*-value also determines the *P* value. The *P* value is the probability of obtaining a result as an extreme of the one that was actually observed, given that the null hypothesis is true. The *F*-value can be calculated as the ratio of mean square for each effect and the mean square for error. While, the *P* value is calculated using the *F*-value in the statistical tool pack of Microsoft Excel. Finally, the F_{crit}-value represents the *F*-statistic for a critical significance level ($\alpha = 0.05$).

TABLE V. Two-factor analysis of the variance for density

Source of variation	*df*	*SS*	*MS*	*F*	*P*	F_{crit}
Rows	9	0.005167	0.000574	560.1684	1.39×10^{-56}	2.032242
Columns	7	0.104215	0.014888	14526.24	1.68×10^{-98}	2.158829
Error	63	6.46×10^{-5}	1.02×10^{-6}			
Total	79	0.109447				

TABLE VI. Two-factor analysis of the variance for refractive index

Source of variation	*df*	*SS*	*MS*	*F*	*P*	F_{crit}
Rows	9	0.000773	8.59×10^{-5}	531.0884	7.28×10^{-56}	2.032242
Columns	7	0.044742	0.006392	39516.43	3.5×10^{-112}	2.158829
Error	63	1.02×10^{-5}	1.62×10^{-7}			
Total	79	0.045525				

TABLE VII. Two-factor analysis of the variance for viscosity

Source of variation	*df*	*SS*	*MS*	*F*	*P*	F_{crit}
Rows	9	23.92058	2.657843	12.90169	2.26×10^{-11}	2.032242
Columns	7	62.35309	8.907584	43.23917	1.06×10^{-21}	2.158829
Error	63	12.97846	0.206007			
Total	79	99.25213				

TABLE VIII. Two-factor analysis of the variance for the coefficient of thermal expansion.

Source of variation	*Df*	*SS*	*MS*	*F*	*P*	F_{crit}
Rows	9	0.127406	0.014156	217.3241	6.37×10^{-44}	2.032242
Columns	7	13.83616	1.976594	30344.3	1.4×10^{-108}	2.158829
Error	63	0.004104	6.51×10^{-5}			
Total	79	13.96767				

As can be seen from Table V, the *F*-values (560.1684 and 14526.24) are bigger than the related F_{crit}-values (2.032242 and 2.158829), while the values of *P* (1.39×10^{-56} and 1.68×10^{-98}) are much smaller than the α value (0.05) for density. Therefore, taking into consideration the above evidence, it could be stated that the experimental density data for the aqueous Na-Phe solutions was statistically correct, and that the effect of concentration and temperature on density is considerable.[42,61] Furthermore, in Tables VI–VIII, the F-values are larger than those of the corresponding F_{crit}-values, while the P-values are much smaller than α for the refractive index, viscosity, and coefficient of thermal expansion. Thus, taking into account the above facts and similar to density, it could be stated that the experimental data for refractive index, viscosity, and coefficient of thermal expansion are factually correct, and significantly dependent on concentration and temperature.[42,61]

CONCLUSIONS

The physical properties, *i.e.*, density, refractive index and viscosity, of aqueous solutions of the sodium salt of L-phenylalanine (Na-Phe) were experimentally measured over a mass fraction range of 0.05 to 0.40 and temperatures 298.15–343.15 K. The experimental values of density, refractive index, and viscosity were found to decrease as the temperature increased (at any fixed concentration), and the isothermal values increased as the concentration of amino acid salt increased. Upon increasing the Na-Phe concentration, intermolecular interactions (van der Waals dispersion forces and dipole–dipole interactions) and H-bonding between the water and Na-Phe molecules also increased. While, with increasing solution temperature, the intermolecular interactions between them decreased. In case of the coefficient of thermal expansion, a slight increment in the values was observed with increasing temperature and concentration. The experimental data of density and refractive index were represented using a modified equation used by Graber, whereas the viscosity data were represented using an applied modified VTF equation. The applied correlations were dependent on both temperature and concentration of aqueous Na-Phe solutions for the corresponding physical property. An evaluation of statistical parameters such as R^2, *RMSE*, *SD*, *AAD* and *ARD* was performed, and the corresponding values of the parameters were found to be satisfactory. An additional analysis in terms of ANOVA was realized in order to understand better the statistical analysis. Thus, the reported data of the investigated physical properties could be useful for an understanding of the molecular interactions in aqueous amino acid salt solutions at different concentrations and temperatures for the CO_2 absorption process.

SUPPLEMENTARY MATERIAL

Density, refractive index and viscosity data, as well as relative error distribution plots, are available at the pages of journal website: http://www.shd.org.rs/JSCS/, or from the corresponding author on request.

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ИЗВОД

ЕКСПЕРИМЕНТАЛНО МЕРЊЕ И ПРЕДВИЂАЊЕ ФИЗИЧКИХ СВОЈСТАВА ВОДЕНОГ РАСТВОРА НАТРИЈУМОВЕ СОЛИ L-ФЕНИЛАЛАНИНА

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У овом раду су испитивана физичка својства: густина, индекс рефракције и вискозност воденог раствора натријумове соли L-фенилаланина (Na-Phe). Поменута својства су одређена за растворе са следећим масеним уделима Na-Phe: 0,05; 0,10; 0,15; 0,20; 0,25; 0,30; 0,35; и 0,40, у опсегу температуре од 298,15 до 343,15 K, на атмосферском притиску. Анализа експерименталних резултата је показала да се вредности густине, индекса рефракције и вискозности раствора смањују са порастом температуре при истој концентрацији Na-Phe. С друге стране, вредности се повећавају са порастом концентрације на истој температури. Резултати за густину раствора су коришћени за процену коефицијента термичког ширења. Коефицијент термичког ширења слабо расте са порастом температуре и концентрације раствора. Вредности густине и индекса рефракције су корелисане једначинама модификованог Graber модела док су вредности вискозности корелисане једначинама модела Vogel–Tamman–Fulcher (VTF). У раду је изведена квантитативна анализа утицаја температуре и концентрације раствора у свим случајевима.

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REFERENCES

1. J. B. Holst, G. F. Versteeg, D. W. F. Brilman, J. A. Hogendoorn, *Chem. Eng. Sci.* **64** (2009) 59
2. J.-A. Lim, D. H. Kim, Y. Yoon, S. K. Jeong, K. T. Park, S. C. Nam, *Energy Fuel* **26** (2012) 3910
3. IEA *World Energy Investment Outlook*, IEA Publications, 2012
4. B. P. Mandal, S. S. Bandyopadhyay, *Chem. Eng. Sci.* **61** (2006) 5440
5. P. W. Derks, K. J. Hogendoorn, G. F. Versteeg, *J. Chem. Eng. Data* **50** (2005) 1947
6. R. Idem, M. Wilson, P. Tontiwachwuthikul, A. Chakma, A. Veawab, A. Aroonwilas, D. Gelowitz, *Ind. Eng. Chem. Res.* **45** (2005) 2414
7. B. P. Mandal, M. Guha, A. K. Biswas, S. S. Bandyopadhyay, *Chem. Eng. Sci.* **56** (2001) 6217
8. A. M. Shariff, M. S. Shaikh, M. A. Bustam, S. Garg, N. Faiqa, A. Aftab, *Procedia Eng.* **148** (2016) 444
9. S. Kadiwala, A. V. Rayer, A. Henni, *Fluid Phase Equilib.* **292** (2010) 20
10. R. Steeneveldt, B. Berger, T. A. Torp, *Chem. Eng. Res. Des.* **84** (2006) 739
11. N. MacDowell, N. Florin, A. Buchard, J. Hallett, A. Galindo, G. Jackson, C. S. Adjiman, C. K. Williams, N. Shah, P. Fennell, *Energy Environ. Sci.* **3** (2010) 1645
12. A. A. Olajire, *Energy* **35** (2010) 2610
13. J. Kittel, R. Idem, D. Gelowitz, P. Tontiwachwuthikul, G. Parrain, A. Bonneau, *Energy Procedia* **1** (2009) 791
14. S. Ma'mun, H. F. Svendsen, K. A. Hoff, O. Juliussen, *Energy Convers. Manage.* **48** (2007) 251

15. M. S. Shaikh, A. M. Shariff, M. A. Bustam, G. Murshid, *J. Chem. Eng. Data* **59** (2014) 362
16. A. F. Ciftja, A. Hartono, H. F. Svendsen, *Energy Procedia* **37** (2013) 1597
17. H. Knuutila, U. E. Aronu, H. M. Kvamsdal, A. Chikukwa, *Energy Procedia* **4** (2011) 1550
18. S. Garg, A. M. Shariff, M. S. Shaikh, B. Lal, A. Aftab, N. Faiqa, *Chem. Eng. Res. Des.* **113** (2016)
19. S. Garg, A. M. Shariff, M. S. Shaikh, B. Lal, A. Aftab, N. Faiqa, *J. Nat. Gas Sci. Eng.* **34** (2016) 864
20. U. E. Aronu, H. F. Svendsen, K. A. Hoff, *Int. J. Greenhouse Gas Control* **4** (2010) 771
21. E. S. Hamborg, J. P. M. Niederer, G. F. Versteeg, *J. Chem. Eng. Data* **52** (2007) 2491
22. P. S. Kumar, J. A. Hogendoorn, G. F. Versteeg, P. H. M. Feron, *AIChE J.* **49** (2003) 203
23. A. F. Portugal, P. W. J. Derks, G. F. Versteeg, F. D. Magalhães, A. Mendes, *Chem. Eng. Sci.* **62** (2007) 6534
24. U. E. Aronu, E. T. Hessen, T. Haug-Warberg, K. A. Hoff, H. F. Svendsen, *Energy Procedia* **4** (2011) 109
25. S. Garg, A. Shariff, M. Shaikh, B. Lal, A. Aftab, N. Faiqa, *Ind. J. Sci. Technol.* **9** (2016), doi: 10.17485/ijst/2016/v9i29/92903
26. A. Hartono, U. E. Aronu, H. F. Svendsen, *Energy Procedia* **4** (2011) 209
27. A. Nuchitprasittichai, S. Cremaschi, *Comput. Chem. Eng.* **35** (2011) 1521
28. S. Lee, S.-I. Choi, S. Maken, H.-J. Song, H.-C. Shin, J.-W. Park, K.-R. Jang, J.-H. Kim, *J. Chem. Eng. Data* **50** (2005) 1773
29. M. S. Shaikh, A. M. Shariff, M. A. Bustam, G. Murshid, *J. Chem. Eng. Data* **58** (2013) 634
30. D. Kang, S. Park, H. Jo, J. Min, J. Park, *J. Chem. Eng. Data* **58** (2013) 1787
31. M. E. Majchrowicz, D. W. F. Brilman, M. J. Groeneveld, *Energy Procedia* **1** (2009) 979
32. G. Murshid, A. M. Shariff, L. K. Keong, M. A. Bustam, *J. Chem. Eng. Data* **56** (2011) 2660
33. M. S. Shaikh, A. M. Shariff, M. A. Bustam, G. Murshid, *Chin. J. Chem. Eng.* **23** (2015) 536
34. A. B. Knežević-Stevanović, J. D. Smiljanić, S. P. Šerbanović, I. R. Radović, M. L. Kijevčanin, *J. Serb. Chem. Soc.* **79** (2014) 77
35. O. Ciocirlan, O. Iulian, *J. Serb. Chem. Soc.* **74** (2009) 317
36. I. R. Radović, M. L. Kijevčanin, A. Ž. Tasić, B. D. Đorđević, S. P. Šerbanović, *J. Serb. Chem. Soc.* **74** (2009) 1303
37. O. Ciocirlan, O. Iulian, *J. Serb. Chem. Soc.* **73** (2008) 73
38. C. K. Foo, C. Y. Leo, R. Aramesh, M. K. Aroua, N. Aghamohammadi, M. S. Shafeeyan, A. Shamiri, *J. Mol. Liq.* **209** (2015) 596
39. S. S. Navarro, R. B. Leron, A. N. Soriano, M.-H. Li, *J. Chem. Thermodyn.* **78** (2014) 23
40. A. A. R. Garcia, R. B. Leron, A. N. Soriano, M.-H. Li, *J. Chem. Thermodyn.* **81** (2015) 136
41. L.-A. Tirona, R. B. Leron, A. N. Soriano, M.-H. Li, *J. Chem. Thermodyn.* **77** (2014) 116
42. M. S. Shaikh, A. M. Shariff, M. A. Bustam, G. Murshid, *Chem. Eng. Res. Des.* **102** (2015) 378
43. J. N. Spencer, W. S. Wolbach, J. W. Hovick, L. Ansel, K. J. Modarress, *J. Solution Chem.* **14** (1985) 805
44. K. W. Raymond, *General Organic and Biological Chemistry*, Wiley, Hoboken, NJ, 2009
45. M. M. Taib, T. Murugesan, *J. Chem. Eng. Data* **57** (2011) 120
46. G. Murshid, A. M. Shariff, K. K. Lau, M. A. Bustam, F. Ahmad, *J. Chem. Eng. Data* **57** (2011) 133
47. S. M. Shuaib, A. M. Shariff, M. A. Bustam, G. Murshid, *J. Serb. Chem. Soc.* **79** (2014) 719
48. F. Chemat, H. J. You, K. Muthukumar, T. Murugesan, *J. Mol. Liq.* **212** (2015) 605
49. M. Bishop, G. H. Locket, *Introduction to Chemistry*, Benjamin Cummings, San Francisco, CA, 2002

50. T. A. Graber, H. R. Galleguillos, C. Céspedes, M. E. Taboada, *J. Chem. Eng. Data* **49** (2004) 1254
51. P.-Y. Lin, A. N. Soriano, R. B. Leron, M.-H. Li, *J. Chem. Thermodyn.* **42** (2010) 994
52. G. S. Fulcher, *J. Am. Ceram. Soc.* **8** (1925) 339
53. F. Civan, *Chem. Eng. Prog.* **104** (2008) 46
54. Y.-P. Hsieh, R. B. Leron, A. N. Soriano, A. R. Caparanga, M.-H. Li, *J. Chem. Eng. Jpn.* **45** (2012) 939
55. M. M. Akbar, T. Murugesan, *J. Mol. Liq.* **169** (2012) 95
56. M. S. Altuwaim, K. H. A. E. Alkhaldi, A. S. Al-Jimaz, A. A. Mohammad, *J. Chem. Eng. Data* **59** (2014) 1955
57. A. Muhammad, M. I. A. Mutalib, C. D. Wilfred, T. Murugesan, A. Shafeeq, *J. Chem. Eng. Data* **53** (2008) 2226
58. A. Muhammad, M. I. A. Mutalib, T. Murugesan, A. Shafeeq, *J. Chem. Eng. Data* **54** (2009) 2317
59. K. Golzar, S. Amjad-Iranagh, H. Modarress, *Ind. Eng. Chem. Res.* **53** (2014) 7247
60. E. Ahmadinia, M. Zargar, M. R. Karim, M. Abdelaziz, P. Shafigh, *Mater. Des.* **32** (2011) 4844
61. R. Afshar Ghotli, A. R. Abdul Aziz, I. M. Atadashi, D. B. Hasan, P. S. Kong, M. K. Aroua, *J. Ind. Eng. Chem.* **21** (2015) 1039.