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SUPPLEMENTARY MATERIAL TO

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

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TABLE S-I. Specifications of the chemicals used; source: Merck

Chemical name	Chemical formula	Purity, %	Molar mass, g
L-Phenylalanine	$C_9H_{11}NO_2$	≥99	165.19
Sodium hydroxide	NaOH	≥99	39.99
Double distilled water	H_2O	≥99	18.01

Calibration of the apparatus

Prior to the measurement of the physical properties of the Na-Phe solutions, all the corresponding equipment was calibrated to ensure consistency in the experimental results and reliability of the data. Pure water was used as a standard for calibration of the equipment. A comparison of the obtained experimental data for the physical properties of pure water with literature data is presented in Table S-II together with the values of the average relative deviation (*ARD*). The deviation values in density, refractive index and viscosity were 0.0127, 0.0004 and 0.1781, respectively. Deviation between experimental and literature values may be due to differences in purity, measuring equipment, and methods. The deviation values in Table S-II confirm proper calibration of the equipment and ensure reliability of the data.

Density measurement

A digital Anton Paar density meter (DMA-4500 M) was used to measure the density of aqueous Na–Phe solutions. The apparatus has a measuring precision of ± 5×10^{-5} g cm^{-3}. The density meter uses the principle of an oscillating U-tube. Each sample of the aqueous amino acid salt was fed into the U-shaped tube that was electronically agitated to oscillate at its specific frequency. This specific frequency changes with the density of the sample taken. Using thorough investigation and proper adjustment of the specific frequency, the density of the sample was measured. The measuring tube was regularly thermo-stated because the density values depend highly on temperature. The equipment was calibrated before each run with pure water. The data reported were the average of three measurements. The estimated uncertainty in density and temperature data was ±7×10^{-5} g cm^{-3} and ±0.01 K, respectively.

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Refractive index measurement

A digital Anton Paar refractometer (Abbemet, model WR) with measuring precision of $\pm 4\times10^{-5}$, was used to measure the refractive index of the aqueous Na-Phe solutions. It has powerful built-in Peltier temperature control system that provides fast heating and cooling rates with an accuracy of ±0.03 K. For the measurements, the samples were placed onto the prism using a pipette. The shape of the measuring vial ensures minimum evaporation of the sample, and prevents a sample with a low surface tension from flowing apart. A minimum--stray light beam was directed from the bottom of the prism at different angles of reflection and the built-in microprocessor spontaneously determined the refractive index of the sample. The equipment was calibrated using pure water at the end of each experiment. The experimental uncertainties in the refractive index and temperature were $\pm6\times10^{-5}$ and ±0.03 K, respectively.

Viscosity measurements

A digital Anton Paar microviscometer (Lovis-2000M) was used to measure the viscosity of the aqueous Na-Phe solutions. This rolling-ball viscometer employs an established measuring principle in accordance with Höppler, DIN 53015 and ISO 12058. A ball rolls through a sample-filled capillary that is inclined at a defined angle. Three inductive sensors measure the rolling time of the ball through transparent or opaque samples between defined marks. The viscometer has an implicit Pt-100 temperature sensor for temperature regulation and measurement with a built-in Peltier temperature control system for faster heating and cooling rates. Calibration with pure water was performed before and after each experiment. The measuring precision of equipment for viscosity was $\pm5\times10^{-3}$ mPa s. The reported values of viscosities were the average of three measurements. The estimated experimental uncertainties of viscosity and temperature were found to be $\pm7\times10^{-3}$ mPa s and ±0.02 K, respectively.

TABLE S-II. Comparison of physical properties of pure water with literature data

T / K	ρ / g cm^{-3}		n_D		η / mPa s	
	This work	Literature[1]	This work	Literature[1]	This work	Literature[1]
303.15	0.99587	0.9956	1.331882	1.33188	0.7972	0.798
308.15	0.99425	0.9940	1.331236	1.33124	0.7193	0.719
313.15	0.99243	0.9923	1.330534	1.33053	0.6536	0.654
318.15	0.99043	0.9903	1.329731	1.32974	0.5955	0.595
323.15	0.98826	0.9882	1.328892	1.32890	0.5473	0.546
328.15	0.98592	0.9859	1.327983	1.32799	0.5043	0.506
333.15	0.98342	0.9834	1.327034	1.32704	0.4678	0.466
ARD / %	–	0.0127	–	0.0004	–	0.1781

TABLE S-III. Density data for aqueous solutions of the sodium salt of L-phenylalanine (ρ / g cm^{-3})

T / K	w							
	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40
298.15	1.01297	1.02913	1.04705	1.06274	1.08018	1.09758	1.11217	1.12691
303.15	1.01135	1.02729	1.04495	1.06042	1.07764	1.09485	1.10933	1.12393
308.15	1.00954	1.02528	1.04272	1.05798	1.07501	1.09204	1.10640	1.12031
313.15	1.00754	1.02311	1.04034	1.05542	1.07227	1.08915	1.10339	1.11779
318.15	1.00538	1.02080	1.03784	1.05275	1.06944	1.08618	1.10033	1.11463
323.15	1.00307	1.01835	1.03522	1.04998	1.06653	1.08314	1.09720	1.11142
328.15	1.00061	1.01577	1.03249	1.04711	1.06353	1.08003	1.09400	1.10815
333.15	0.99801	1.01305	1.02964	1.04414	1.06044	1.07685	1.09074	1.10482
338.15	0.99528	1.01023	1.02669	1.04108	1.05728	1.07359	1.08741	1.10144
343.15	0.99247	1.00728	1.02364	1.03793	1.05403	1.07025	1.08402	1.09800

TABLE S-IV. Refractive index data for aqueous solutions of the sodium salt of L-phenylalanine

T / K	w							
	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40
298.15	1.34231	1.35229	1.36299	1.37309	1.38403	1.39554	1.40536	1.41603
303.15	1.34164	1.35155	1.36216	1.37219	1.38298	1.39443	1.40418	1.41487
308.15	1.34090	1.35074	1.36129	1.37125	1.38198	1.39335	1.40301	1.41365
313.15	1.34010	1.34988	1.36035	1.37026	1.38089	1.39226	1.40183	1.41243
318.15	1.33926	1.34898	1.35938	1.36922	1.37982	1.39108	1.40062	1.41117
323.15	1.33838	1.34804	1.35837	1.36817	1.37871	1.38990	1.39942	1.40991
328.15	1.33744	1.34705	1.35731	1.36706	1.37756	1.38876	1.39821	1.40867
333.15	1.33645	1.34601	1.35624	1.36595	1.37639	1.38753	1.39696	1.40738
338.15	1.33542	1.34493	1.35515	1.36479	1.37517	1.38625	1.39569	1.40607
343.15	1.33434	1.34381	1.35401	1.36357	1.37394	1.38499	1.39435	1.40472

TABLE S-V. Viscosity data for aqueous solutions of the sodium salt of L-phenylalanine (η / mPa s)

T / K	w							
	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40
298.15	0.991	1.142	1.476	1.725	2.258	2.963	4.238	6.254
303.15	0.885	1.013	1.302	1.511	1.970	2.548	3.597	5.210
308.15	0.796	0.906	1.157	1.336	1.728	2.213	3.089	4.391
313.15	0.721	0.817	1.038	1.190	1.530	1.948	2.679	3.740
318.15	0.656	0.740	0.936	1.069	1.366	1.723	2.342	3.259
323.15	0.602	0.675	0.850	0.966	1.226	1.534	2.072	2.794
328.15	0.554	0.619	0.776	0.878	1.107	1.375	1.840	2.446
333.15	0.513	0.571	0.712	0.802	1.007	1.240	1.645	2.158
338.15	0.477	0.529	0.657	0.737	0.920	1.125	1.480	1.932
343.15	0.446	0.492	0.609	0.679	0.844	1.026	1.340	1.729

TABLE S-VI. Fitting parameters of Eq. (7) for the coefficient of thermal expansion; $n = 10$

w	Parameter	
	C_0	$C_1 \times 10^4$
0.05	1.150	–4.579
0.10	1.175	–4.869
0.15	1.203	–5.213
0.20	1.228	–5.522
0.25	1.254	–5.816
0.30	1.279	–6.074
0.35	1.299	–6.259
0.40	1.319	–6.430

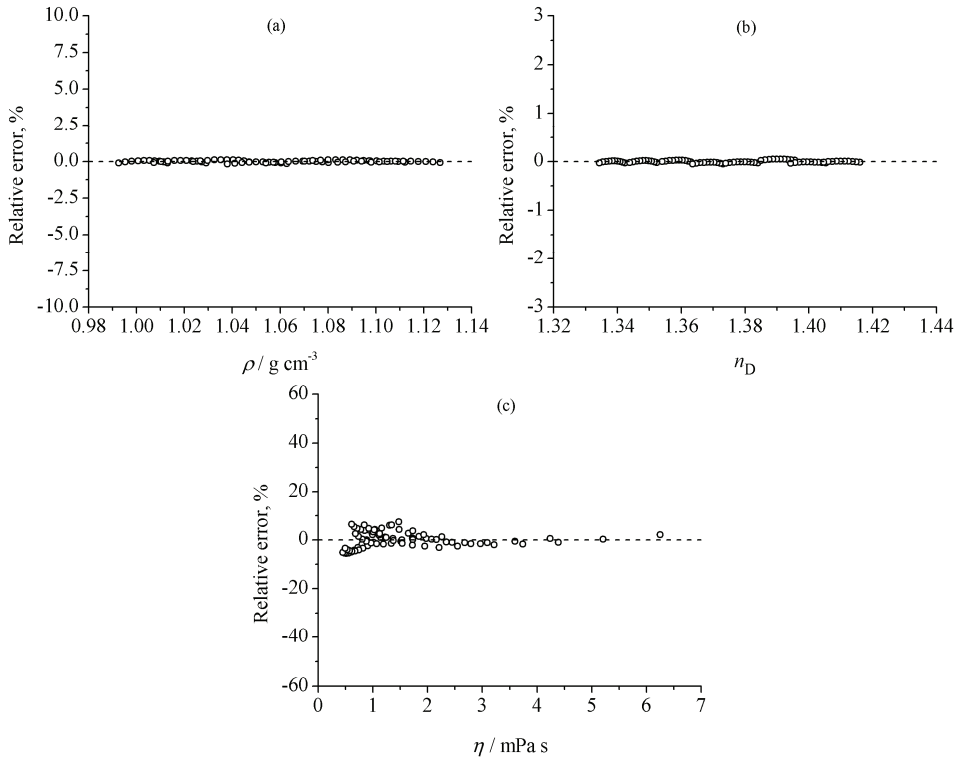

Fig. S-1. Relative error distribution: a) density; b) refractive index; c) viscosity.

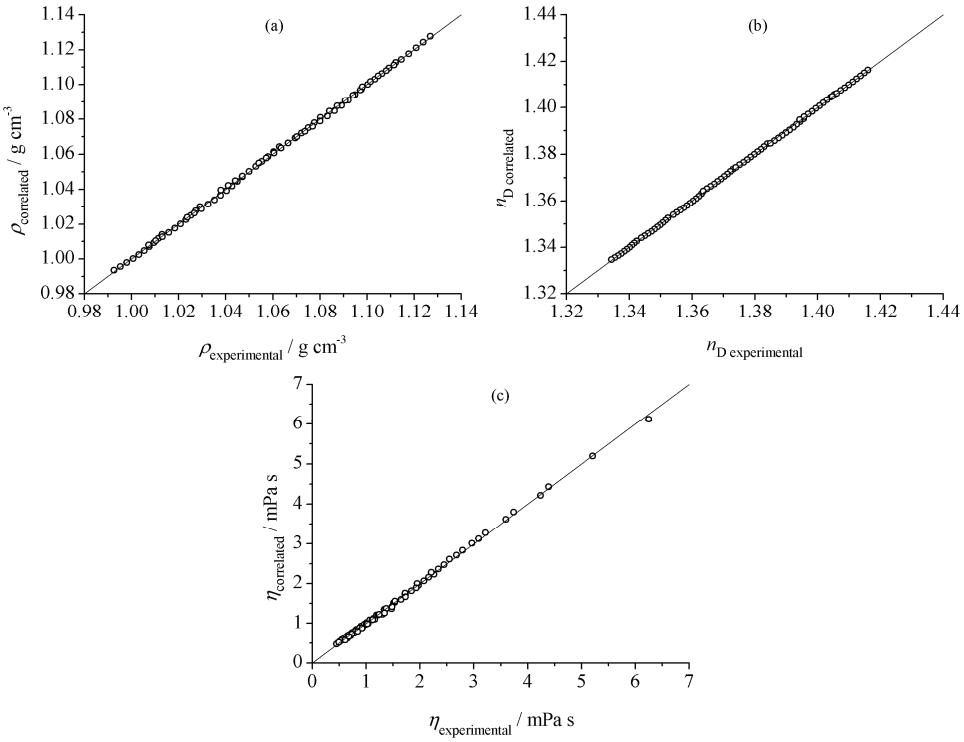

Fig. S-2. Cross-plots of experimental and correlated data: a) density; b) refractive index; c) viscosity.

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