JOURNAL OF
CHEMICAL &
ENGINEERING
DATA

ARTICLE

pubs.acs.org/jced

Densities, Viscosities [from (278.15 to 318.15) K], and Electrical Conductivities (at 298.15 K) of Aqueous Solutions of Choline Chloride and Chloro-Choline Chloride

Saadia Shaukat and Richard Buchner*

Institut für Physikalische und Theoretische Chemie, Universität Regensburg, D-93040 Regensburg, Germany

S *Supporting Information*

ABSTRACT: Data for the electrical conductivity (at 298.15 K), density, and viscosity [both at (278.15, 288.15, 298.15, 308.15, and 318.15) K] of aqueous solutions of choline chloride (ChCl) and chloro-choline chloride (Cl-ChCl) are reported for solute molalities $m \lesssim 2.0\ \text{mol}\cdot\text{kg}^{-1}$ (ChCl) and $\lesssim 2.1\ \text{mol}\cdot\text{kg}^{-1}$ (Cl-ChCl), respectively. From the densities apparent molar volumes were calculated, and the limiting partial molar volumes and Hepler's constants of ChCl(aq) and Cl-ChCl(aq) were evaluated. From the viscosities Arrhenius activation energies of viscous flow were determined. While apparent molar volumes suggest at best weak ion pairing for ChCl(aq) and Cl-ChCl(aq), the Walden product obtained for 25 °C hints at significant ion−ion interactions and/or changes in ion hydration with increasing concentration.

INTRODUCTION

Choline (vitamin B4, the (2-hydroxy)ethyltrimethylammonium cation) is an important biological ion and designated as to be an essential part of our daily diet.[1] Choline (Ch^+) plays several key functions in the human body as it keeps the constituency of cell membranes, is involved in cholinergic neurotransmission,[2] and is a major component of pulmonary surfactants.[3] Recently, choline-based ionic liquids have attracted increased interest,[4] as have anionic surfactants with Ch^+ as the counterion.[5,6] Chloro-choline, (the (2-chloro)ethyltrimethylammonium cation, Cl-Ch^+) is active as a plant growth regulator,[7] and its salts are used as an additive to animal feed.[8]

The present study reports some physical properties of aqueous solutions of choline chloride (ChCl) and chloro-choline chloride (Cl-ChCl), namely, electrical conductivity, κ, at 298.15 K, as well as density, ρ, and dynamic viscosity, η, at (278.15, 288.15, 298.15, 308.15, and 318.15) K in the concentration (molality) range ($0.02 \lesssim m/\text{mol}\cdot\text{kg}^{-1} \lesssim 2.1$).

EXPERIMENTAL SECTION

Materials. Prior to use, ChCl (Sigma-Aldrich, 98% purity) and Cl-ChCl (Sigma-Aldrich, 98 % purity) were dried at 40 °C in vacuum for about 72 h using P_2O_5 (Sicapent, Merck) as a desiccant and then stored under dry N_2 atmosphere. Solutions were prepared by weight without buoyancy corrections (thus a relative uncertainty in solute molality, m, of ± 0.002) using Millipore water having $\kappa < 2\cdot10^{-5}\ \text{S}\cdot\text{m}^{-1}$.

Table 1. Electrical Conductivities, κ, of Aqueous Solutions of ChCl and Cl-ChCl at 298.15 K

ChCl		Cl-ChCl	
m	κ	m	κ
$\text{mol}\cdot\text{kg}^{-1}$	$\text{S}\cdot\text{m}^{-1}$	$\text{mol}\cdot\text{kg}^{-1}$	$\text{S}\cdot\text{m}^{-1}$
0.0272	0.279	0.0277	0.265
0.0500	0.492	0.0514	0.490
0.1000	0.919	0.1003	0.898
0.2500	2.03	0.2497	1.97
0.3500	2.67	0.3502	2.58
0.5000	3.55	0.5001	3.36
0.6500	4.37	0.6509	4.10
0.7500	4.79	0.7498	4.51
0.9000	5.44	0.8997	5.07
1.2048	6.54	0.9998	5.42
1.5047	7.43	1.2117	6.08
1.9945	8.53	1.5070	6.81
		1.9980	7.67

Electrical Conductivity. Conductivity measurements for ChCl(aq) were performed at 298.15 K with the Wheatstone-bridge equipment described previously,[9,10] using a home-built precision thermostat with temperature stability of <0.003 K. For Cl-ChCl(aq) a computer-controlled setup was used consisting of a Huber Unistat 705 as the thermostat (temperature stability <0.005 K), a high-precision LCR bridge (HAMEG HM8118) for resistance measurement (relative uncertainty ≤0.0005), and a switchboard to address the three two-electrode capillary cells mounted on the thermostat lid. Parasitic impedances were eliminated by an open/short calibration of LCR bridge and switchboard prior to each measurement. The cells with cell constants C ranging from (25 to 360) cm^{-1} were calibrated with KCl(aq).[11] Measurement temperatures were recorded with an uncertainty of ± 0.01 K with a NIST traceable Pt-resistance thermometer (ASL). To

Special Issue: Kenneth N. Marsh Festschrift

Received: August 1, 2011
Accepted: September 29, 2011
Published: October 20, 2011

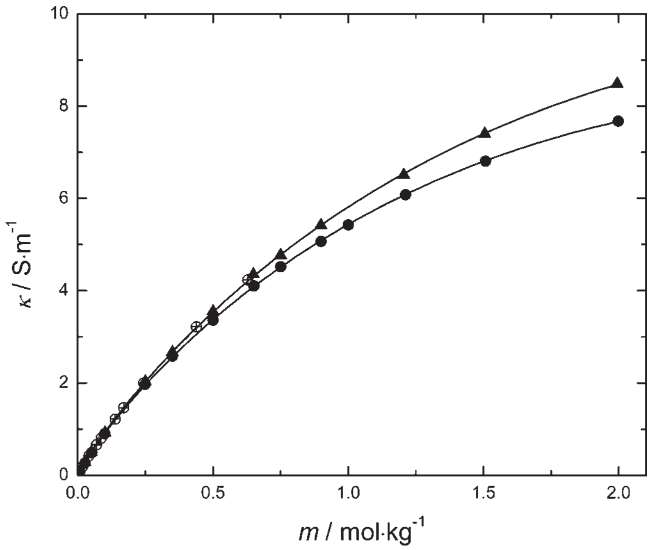

Figure 1. Electrical conductivities, κ, of aqueous solutions of ChCl (▲, this work; ⊕, ref 15) and Cl-ChCl (●) at 298.15 K as a function of solute molality, m. Solid lines represent fits with the Casteel—Amis equation, eq 1.

Table 2. Maximum Conductivity, $\kappa_{\max}$, Corresponding Electrolyte Molality, $m_{\max}$, and Shape Parameter, a, of Equation 1 ($b = 0$ fixed) for Aqueous Solutions of ChCl and Cl-ChCl at 298.15 K. Also Included Is the Corresponding Standard Error of the Fit, σ_{fit}

	$\kappa_{\max}$ / $\text{S}\cdot\text{m}^{-1}$	$m_{\max}$ / $\text{mol}\cdot\text{kg}^{-1}$	a	σ_{fit} / $\text{S}\cdot\text{m}^{-1}$
ChCl	9.75 ± 0.10	3.71 ± 0.09	0.891 ± 0.008	0.02
Cl-ChCl	8.42 ± 0.06	3.30 ± 0.06	0.883 ± 0.007	0.02

Table 3. Densities, ρ, of Aqueous Solutions of ChCl and Cl-ChCl at Molality, m, and Temperature, T

m	$\rho/\text{kg}\cdot\text{m}^{-3}$ at T/K				
$\text{mol}\cdot\text{kg}^{-1}$	278.15	288.15	298.15	308.15	318.15
			ChCl		
0[a]	999.964	999.099	997.043	994.029	990.208
0	999.961	999.092	997.036	994.023	990.206
0.0540	1000.967	1000.031	997.931	994.893	991.063
0.1087	1001.952	1000.950	998.810	995.745	991.902
0.2554	1004.503	1003.333	1001.088	997.961	994.085
0.5004	1008.705	1007.266	1004.844	1001.614	997.683
0.6512	1011.014	1009.433	1006.921	1003.633	999.672
0.7484	1012.676	1010.996	1008.420	1005.091	1001.109
1.2030	1019.283	1017.228	1014.403	1010.921	1006.860
1.5035	1022.746	1020.505	1017.560	1014.000	1009.901
1.9924	1028.852	1026.308	1023.157	1019.473	1015.308
			Cl-ChCl		
0.0506	1001.453	1000.522	998.426	995.387	991.452
0.1009	1002.888	1001.900	999.762	996.694	992.837
0.2364	1006.793	1005.646	1003.397	1000.252	996.273
0.5010	1013.917	1012.479	1010.021	1006.724	1002.683
0.6523	1017.877	1016.276	1013.698	1010.315	1006.203
0.7529	1020.456	1018.745	1016.090	1012.650	1008.516
1.1995	1031.176	1029.024	1026.042	1022.358	1018.058
1.4973	1038.126	1035.683	1032.481	1028.632	1024.208
1.9862	1048.245	1045.386	1041.866	1037.775	1033.173

[a] Reference 16.

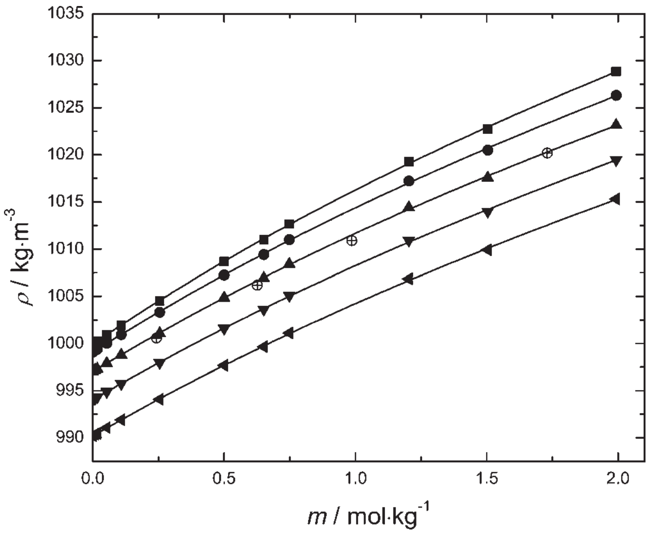

Figure 2. Densities, ρ, of aqueous ChCl as a function of solute molality, m, at (■, 278.15; ●, 288.15; ▲, 298.15; ▼, 308.15 and ◀, 318.15) K. Solid lines represent fits of eq 2 ($Y = \rho$; $n = 3$). For comparison the data (⊕) of Fleming[15] at 298.15 K are included.

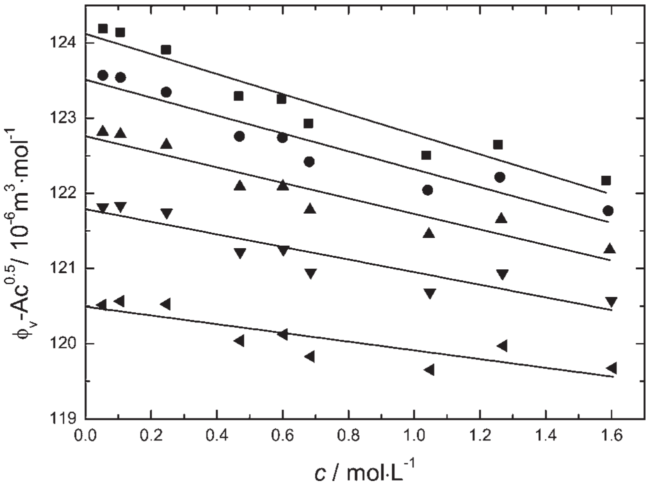

Figure 3. Apparent molar volume, ϕ_V, of ChCl in aqueous solution as a function of salt concentration, c, at (◀, 278.15; ▼, 288.15; ▲, 298.15; ●, 308.15 and ■, 318.15) K. Solid lines represent fits of eq 4.

overcome possible effects of electrode polarization, cell resistance, R, was measured for both setups as a function frequency, ν, in the range $100 \leq \nu/\text{Hz} \leq 10000$. The sample conductivity then was obtained as $\kappa = C/R_\infty$ from the extrapolation $R_\infty = \lim_{\nu\to\infty} R(\nu)$ using the empirical function $R(\nu) = R_\infty + A/\nu^a$; the parameter A is specific to the cell and as expected the exponent a was found to be $0.5 \lesssim a \lesssim 1$.[12] Taking into account all likely sources of error, a relative uncertainty of 0.005 is estimated for κ.

Density. Solution densities, ρ, were measured at (278.15, 288.15, 298.15, 308.15, and 318.15) K with a temperature uncertainty ≤ 0.01 K and stability ≤ 0.002 K using a vibrating-tube densimeter (Anton Paar DMA 5000 M, calibrated by the manufacturer) with a stated uncertainty of $\pm$ 0.005 $\text{kg}\cdot\text{m}^{-3}$ in ρ.

Viscosity. Dynamic viscosities, η, were measured at (278.15, 288.15, 298.15, 308.15, and 318.15) K with a temperature uncertainty ≤ 0.05 K and stability ≤ 0.01 K using an automated rolling-ball viscometer (Anton Paar AMVn). The stated relative uncertainty of the instrument is ≤0.005, although overall errors are probably slightly higher.

RESULTS AND DISCUSSION

Electrical Conductivity. The obtained electrical conductivities are summarized in Table 1 and Figure 1. Consistent with the slightly smaller partial molar volume of this compound (see below) $\kappa(m)$ is always larger for ChCl compared to Cl-ChCl. The dependence of κ on salt molality is well-described by the empirical Casteel–Amis equation[13]

$$\kappa = \kappa_{\max}\left(\frac{m}{m_{\max}}\right)^{a}\exp\left[-bm_{\max}^{2}\left(\frac{m}{m_{\max}}-1\right)^{2}-a\left(\frac{m}{m_{\max}}-1\right)\right] \tag{1}$$

where $\kappa_{\max}$ is the maximum conductivity reached at molality $m_{\max}$ while a and b are shape parameters. Since neither for ChCl(aq) nor for Cl-ChCl(aq) $\kappa_{\max}$ was reached in the investigated concentration range $b = 0$ was assumed in the fit.[14] The resulting parameters are summarized in Table 2.

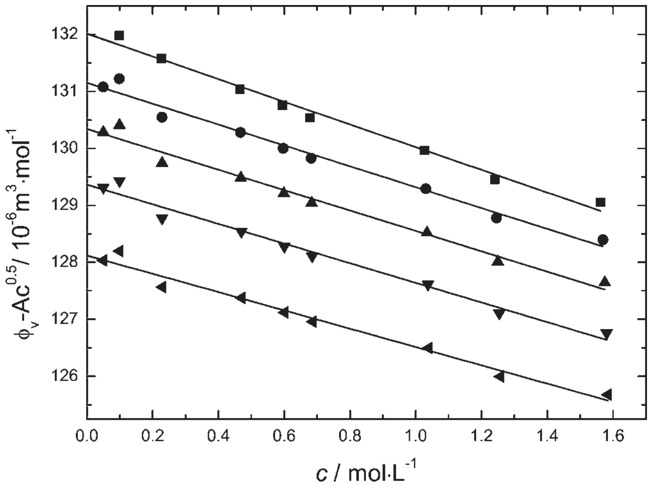

Figure 4. Apparent molar volume, ϕ_v, of Cl-ChCl in aqueous solution as a function of salt concentration, c, at (◀, 278.15; ▼, 288.15; ▲, 298.15; ●, 308.15 and ■, 318.15) K. Solid lines represent fits of eq 4.

To the best of our knowledge literature data for conductivity are only available for ChCl at 298.15 K.[15] As can be seen from Figure 1 the agreement with our conductivities is good with deviations $\delta_\kappa = |\kappa_{\text{fit}} - \kappa_{\text{lit}}| < 0.03\ \text{S}\cdot\text{m}^{-1}$.

Density. The obtained ρ values are given in Table 3, Figure 2 (ChCl), and Figure S1 of the Supporting Information (Cl-ChCl). Also included in Table 3 are literature data[16] for the density of pure water at the investigated temperatures. The latter deviate from our results by 0.007 kg·m^{-3} at maximum, lending credit to the stated reproducibility of the instrument (± 0.005 kg·m^{-3}) and to the quality of the used water sample.

The density data for ChCl and Cl-ChCl at all temperatures can be well-fitted ($\sigma_{\text{fit}} \le 0.12\ \text{kg}\cdot\text{m}^{-3}$ for ChCl and 0.06 kg·m^{-3} for Cl-ChCl) with a polynomial in solute molality

$$Y = \sum_{j=0}^{n} a_j m^j \tag{2}$$

where $Y = \rho$ and $n = 3$. The obtained parameters, a_j, are summarized in Table S1 of the Supporting Information together with the corresponding standard deviation of the fit, σ_{fit}; fit curves are shown in Figures 2 and S1 for ChCl and Cl-ChCl, respectively. Compared to the deviations of the present densities for pure water from corresponding literature data,[16] which do not exceed ≤ 0.007 kg·m^{-3}, the fit standard errors for the solutions are considerably larger. This almost certainly reflects the uncertainty in m. For a comparison of solution densities again only data of Fleming[15] for ChCl(aq) at 298.15 K are available (Figure 2). The agreement is good with relative deviations $\le 5.5\cdot 10^{-4}$.

From ρ the corresponding apparent molar volumes, ϕ_v (Figures 3 and 4), were calculated using the equation[17]

$$\phi_v = \frac{M}{\rho(m)} + \frac{\rho(0) - \rho(m)}{m\rho(0)\rho(m)} \tag{3}$$

where M is the molar mass (ChCl: 0.13962 kg·mol^{-1}; Cl-ChCl: 0.15807 kg·mol^{-1}). According to Redlich and Meyer[18] for electrolyte solutions the dependence of ϕ_v on solute concentration

Table 4. Limiting Partial Molar Volumes, ϕ_v^0, Debye–Hückel Parameters, A_{DH},[20] and Sensitivity Parameters, h, of Equation 4 for Aqueous Solutions of ChCl and Cl-ChCl at Temperature, T. Also Included Are the Corresponding Limiting Apparent Molar Expansibilities, ϕ_E^0

T K	ϕ_v^0 10^{-6} m^3·mol^{-1}	A_{DH}[a] 10^{-6} m^3·L$^{1/2}$·mol$^{-3/2}$	h 10^{-6} m^3·L·mol^{-2}	ϕ_E^0 10^{-6} m^3·mol^{-1}·K^{-1}
		ChCl		
278.15	120.49 ± 0.11	1.5498	− 0.59 ± 0.13	0.137
288.15	121.79 ± 0.11	1.6728	− 0.82 ± 0.13	0.113
298.15	122.76 ± 0.11	1.8332	− 1.01 ± 0.13	0.090
308.15	123.51 ± 0.11	2.0259	− 1.18 ± 0.14	0.066
318.15	124.12 ± 0.12	2.2499	− 1.34 ± 0.14	0.043
		Cl-ChCl		
278.15	128.12 ± 0.07	1.5498	− 1.62 ± 0.09	0.124
288.15	129.37 ± 0.07	1.6728	− 1.71 ± 0.09	0.110
298.15	130.34 ± 0.08	1.8332	− 1.77 ± 0.09	0.096
308.15	131.15 ± 0.08	2.0259	− 1.82 ± 0.09	0.082
318.15	132.01 ± 0.08	2.2499	− 2.00 ± 0.09	0.068

[a] Converted to molarity scale with the water densities of ref 16.

Table 5. Temperature Coefficients, a_i^ϕ ($j = 0, 1, 2$), of Equation 5 for the Limiting Partial Molar Volumes, ϕ_v^0, of ChCl(aq) and Cl-ChCl(aq) and Corresponding Fit Standard Errors, σ_{fit}

	a_0	a_1	a_2	σ_{fit}
	10^{-6} m^3·mol^{-1}	10^{-6} m^{-3}·mol^{-1}·K^{-1}	10^{-6} m^{-3}·mol^{-1}·K^{-2}	10^{-6} m^3·mol^{-1}
ChCl	122.77 ± 0.03	0.0898 ± 0.0014	−0.00117 ± 0.00011	0.04
Cl-ChCl	130.34 ± 0.05	0.0959 ± 0.0023	−0.00071 ± 0.00019	0.07

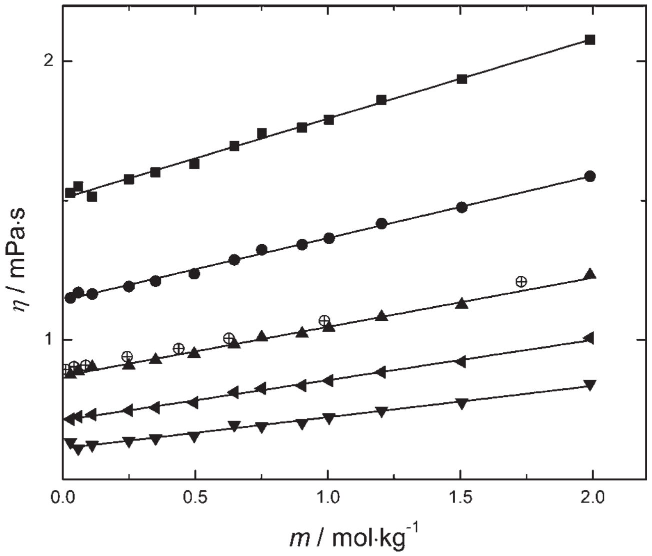

Figure 5. Dynamic viscosities, η, of aqueous ChCl as a function of solute molality, m, at (■, 278.15; ●, 288.15; ▲, 298.15; ◀, 308.15 and ▼, 318.15) K. Solid lines are the linear fits of eq 2 ($Y = \eta$; $n = 1$). For comparison the data (⊕) of Fleming[15] at 298.15 K are included.

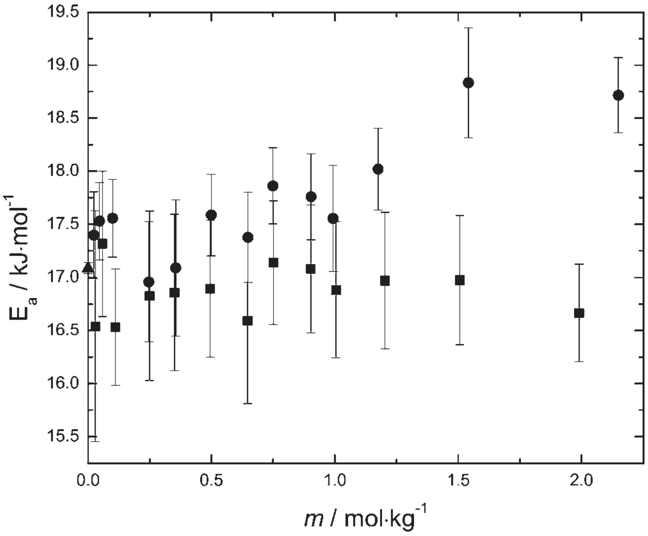

Figure 6. Arrhenius activation energy, E_a, of viscous flow for aqueous solutions of ■, ChCl and ●, Cl-ChCl as a function of solute molality, m. The E_a value of pure water (▲, calculated from the data of ref 24) is also shown.

c ($= \rho(m) \cdot m/(1 + Mm)$) should follow the relation

$$\phi_v = \phi_v^0 + A_{DH}c^{1/2} + hc \tag{4}$$

where ϕ_v^0 is the limiting partial molar volume of the solute and A_{DH} is the Debye−Hückel limiting slope (constant for all 1:1 electrolytes in a given solvent at a certain T). The empirical "deviation parameter", h, of eq 4 is thought to measure ion−ion interactions in the chosen system.[19] The fits obtained with A_{DH} values taken from Archer and Wang[20] (converted to molarity scale) are shown in Figure 3 for ChCl and Figure 4 for Cl-ChCl; the derived limiting partial molar volumes, ϕ_v^0, and h values are summarized in Table 4.

As expected from the larger van der Waals volume of the chlorine atom compared to the OH group, ϕ_v^0(Cl-ChCl) > ϕ_v^0(ChCl). The present result for the limiting partial molar volume of ChCl at 298.15 K, ϕ_v^0(ChCl) = $122.8 \cdot 10^{-6}$ m^3·mol^{-1}, is slightly smaller than the value published by Fleming[15] ($124.9 \cdot 10^{-6}$ m^3·mol^{-1}). This is mainly due to the slightly smaller densities of ref 15, but the different A_{DH} parameters used there also contribute to the difference.

For ChCl and Cl-ChCl ϕ_v^0 increases with increasing temperature according to the relation

$$\phi_v^0 = a_0^\phi + a_1^\phi(T - T_0) + a_2^\phi(T - T_0)^2 \tag{5}$$

where $T_0 = 298.15$ K.[21] The obtained parameters, a_j ($j = 0, ..., 2$), collected in Table 5, permit the calculation of the limiting apparent molar expansibility

$$\phi_E^0 = \left(\frac{\partial \phi_v^0}{\partial T}\right)_p = a_1^\phi + 2a_2^\phi(T - T_0) \tag{6}$$

of ChCl and Cl-ChCl in water (Table 4) and of the corresponding Hepler's constant,[22] $(\partial^2\phi_v^0/\partial T^2)_p = 2a_2^\phi$ ($= (-0.0023 \pm 0.0002) \cdot 10^{-6}$ m^3·mol^{-1}·K^{-2} for ChCl; $(-0.0014 \pm 0.0004) \cdot 10^{-6}$ m^3·mol^{-1}·K^{-2} for Cl-ChCl).

Similar to aqueous NaCl solutions[23] the deviation parameter, h, is negative and decreases with rising temperature for both ChCl(aq) and Cl-ChCl(aq). This suggests that ion pairing is weak and ion−ion interactions decrease further with increasing thermal motions.[23] The rather small concentration dependence of ϕ_v^0 (and thus small $|h|$ values) for ChCl suggests that both ions well fit into the water structure, whereas the fairly negative h for Cl-ChCl may indicate mutual salting-in of the ions, as discussed by Desnoyers and Arel for some n-alkylamine hydrobromides.[17]

Viscosity. Table 6 summarizes the dynamic viscosities, η, determined for ChCl(aq) and Cl-ChCl(aq). To the best of our knowledge only the data of Fleming[15] for ChCl(aq) at 298.15 K are available for comparison (Figure 5). These are slightly larger than the present results with relative deviations $\leq 3.4 \cdot 10^{-2}$.

For ChCl(aq) plots of $\eta = f(m)$ are linear over the entire range of m (Figure 5), whereas a notable curvature was found for Cl-ChCl(aq) (Figure S2 of the Supporting Information). The data

Table 6. Dynamic Viscosities, η, of Aqueous Solutions of ChCl and Cl-ChCl at Molality, m, and Temperature, T

m	η/mPa·s at T/K				
mol·kg^{-1}	278.15	288.15	298.15	308.15	318.15
		ChCl			
0.0293	1.527	1.151	0.875	0.715	0.633
0.0580	1.551	1.170	0.888	0.724	0.610
0.1113	1.515	1.164	0.903	0.732	0.623
0.2495	1.577	1.192	0.908	0.746	0.638
0.3505	1.601	1.211	0.928	0.757	0.646
0.4956	1.631	1.237	0.950	0.774	0.656
0.6473	1.695	1.287	0.984	0.811	0.694
0.7512	1.741	1.323	1.009	0.826	0.690
0.9030	1.762	1.342	1.023	0.835	0.702
1.0049	1.791	1.364	1.043	0.854	0.721
1.2029	1.862	1.417	1.082	0.884	0.747
1.5060	1.936	1.476	1.127	0.921	0.776
1.9896	2.077	1.587	1.234	1.007	0.843
		Cl-ChCl			
0.0236	1.526	1.148	0.907	0.711	0.596
0.0464	1.536	1.156	0.913	0.714	0.595
0.0994	1.555	1.172	0.924	0.722	0.602
0.2464	1.610	1.211	0.955	0.757	0.645
0.3552	1.656	1.241	0.977	0.770	0.660
0.4990	1.712	1.286	1.012	0.793	0.661
0.6479	1.778	1.335	1.047	0.831	0.694
0.7493	1.815	1.362	1.069	0.833	0.691
0.9041	1.914	1.433	1.124	0.879	0.733
0.9927	1.933	1.447	1.133	0.890	0.750
1.1758	2.010	1.502	1.173	0.915	0.759
1.5415	2.298	1.708	1.292	1.005	0.835
2.1484	2.612	1.932	1.493	1.158	0.948

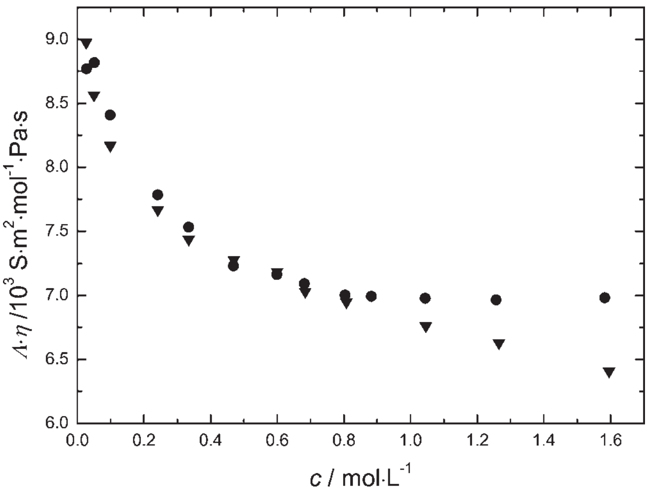

Figure 7. Walden product, $\Lambda\eta$, of aqueous solutions of ▼, ChCl and ●, Cl-ChCl at 298.15 K.

can be well-fitted with eq 2 where $Y = \eta$, $n = 1$ for ChCl, and $n = 2$ for Cl-ChCl. The obtained parameters are summarized in Table 7.

Table 7. Coefficients a_j of Equation 2 ($Y = \eta$) for the Viscosity, η, of Aqueous Solutions of ChCl ($n = 1$) and Cl-ChCl ($n = 2$) at Temperature, T

T	a_0	a_1	a_2
K	mPa·s	mPa·s·kg·mol^{-1}	mPa·s·kg^2·mol^{-2}
		ChCl	
278.15	1.508 ± 0.006	0.286 ± 0.007	
288.15	1.142 ± 0.004	0.223 ± 0.004	
298.15	0.870 ± 0.004	0.176 ± 0.004	
308.15	0.711 ± 0.003	0.144 ± 0.003	
318.15	0.610 ± 0.004	0.112 ± 0.004	
		Cl-ChCl	
278.15	1.516 ± 0.012	0.360 ± 0.029	0.073 ± 0.014
288.15	1.141 ± 0.008	0.268 ± 0.021	0.049 ± 0.010
298.15	0.904 ± 0.003	0.196 ± 0.008	0.036 ± 0.004
308.15	0.800 ± 0.004	0.157 ± 0.009	0.024 ± 0.004
318.15	0.596 ± 0.006	0.134 ± 0.014	0.013 ± 0.007

For liquids and solutions far from the glass-transition temperature, as should be the case for the present samples, the temperature dependence of η is generally well-described by the Arrhenius equation

$$\ln \eta = \ln \eta_\infty + E_a/(RT) \tag{7}$$

where η_∞ is the limiting viscosity for $T \to \infty$, R the gas constant, and E_a the activation energy of viscous flow.

Figure 6 shows the activation energies obtained from the present viscosity data. For ChCl(aq) E_a is essentially independent of solute molality over the entire concentration range, yielding an average value of 16.9 kJ·mol^{-1}, whereas E_a appears to increase linearly for Cl-ChCl(aq). However, these results have to be taken with a grain of salt. Error bars for E_a are rather large, and a close inspection of the fits (Figures S3 and S4 of the Supporting Information) reveals that especially at low concentrations, and more pronounced for ChCl (Figure S3), ln $\eta(T)$ shows a small but significant positive curvature, possibly indicating Vogel–Fulcher–Tamann (VFT) behavior already around room temperature. However, a larger temperature range than that covered in the present investigation [(278.15 to 318.15) K] is required for a thorough determination of the curvature.

According to Walden's rule,[25] $\Lambda\eta$ = constant, the product of viscosity and molar conductivity, Λ (= κ/c), should be independent of concentration as long as ion association is negligible. Since the values obtained for the h parameter of eq 4 suggest only weak ion association it is therefore surprising to find a rather large decrease of $\Lambda\eta$ with increasing m for both ChCl(aq) and Cl-ChCl(aq) (Figure 7). However, it should be kept in mind that also changes in ion solvation with rising concentration may cause deviation from Walden's rule.[26] To clarify this issue, dielectric relaxation studies are currently under way to obtain molecular-level information on ion hydration and association in these systems.

■ CONCLUSIONS

Electrical conductivities (at 298.15 K), densities, and viscosities [in the range (273.15 to 318.15) K] of aqueous solutions of ChCl and Ch-ChCl up to ~2 mol·kg^{-1} are reported.

Comparable literature data are only available from Fleming[15] for ChCl at 298.15 K. Generally, the agreement with the present results is good.

Conductivities are well fitted by the Casteel—Amis equation, eq 1, whereas low-order polynomials were used to fit $\rho(m)$ and $\eta(m)$. Apparent molar volumes, ϕ_v, calculated from ρ are well-described by the Redlich—Meyer approach, eq 4. The obtained sensitivity parameter, h, suggests at best weak ion pairing for ChCl and Cl-ChCl, whereas the Walden product at 298.15 K points at significant ion—ion interactions and/or changes in ion hydration with rising concentration. The small but notable difference in the h values of ChCl(aq) and Cl-ChCl(aq), as well as the different concentration dependence of the activation energy of viscous flow might indicate that solvation effects predominate.

■ ASSOCIATED CONTENT

Ⓢ Supporting Information. Coefficients of eq 2 (Table S1), densities and dynamic viscosities of aqueous solutions of Cl-ChCl as a function of solute molality (Figures S1 and S2), and Arrhenius plots of aqueous solutions of ChCl and Cl-ChCl (Figures S3 and S4). This material is available free of charge via the Internet at http://pubs.acs.org.

■ AUTHOR INFORMATION

Corresponding Author

*E-mail: richard.buchner@chemie.uni-regensburg.de.

Funding Sources

The higher Education Commission of Pakistan (HEC) is gratefully acknowledged for funding S.S.'s stay in Germany.

■ ACKNOWLEDGMENT

The authors thank W. Kunz for providing laboratory facilities in Regensburg.

■ REFERENCES

(1) Food and Nutrition Board, Institute of Medicine. *Dietary Reference Intakes for Thiamin, Riboflavin, Niacin, Vitamin B6, Folate, VitaminB12, Pantothenic Acid, Biotin, and Choline*; National Academic Press: Washington, DC, 1998.

(2) Zeisel, S. H.; Blusztajn, J. K. Choline and Human Nutrition. *Ann. Rev.* **1994**, *14*, 269–296.

(3) Rooney, S. A. Lung Surfactant. *Environ. Health Perspect.* **1984**, *55*, 205–226.

(4) Abbott, A. P.; Barron, J. C.; Ryder, K. S.; Wilson, D. Eutectic-Based Ionic Liquids with Metal-Containing Anions and Cations. *Chem.—Eur. J.* **2007**, *13*, 6495–6501.

(5) Klein, R.; Touraud, D.; Kunz, W. Choline Carboxylate Surfactants: Biocompatible and Highly Soluble in Water. *Green Chem.* **2008**, *10*, 433–435.

(6) Klein, R.; Kellermeier, M.; Drechsler, M.; Touraud, D.; Kunz, W. Solubilisation of Stearic Acid by the Organic Base Choline Hydroxide. *Colloids Surf., A* **2009**, *338*, 129–134.

(7) Tolbert, N. E. (2-Chloroethyl)trimethylammonium Chloride and Related Compounds as Plant-Growth Substances. I. Chemical structure and bioassay. *J. Biol. Chem.* **1960**, *235*, 475–479.

(8) Gultom, D.; Songsang, A.; Meulen, U. T. The Effect of Chlorocholine Chloride (CCC) Inclusion in the Diets of Growing Hens on Growth Rate, Oestrogen Levels and the Onset of Lay. *J. Anim. Physiol. Anim. Nutr.* **2001**, *85*, 1–8.

(9) Barthel, J.; Graml, H.; Neueder, R.; Turq, P.; Bernard, O. Electrolyte Conductivity From Infinite Dilution to Saturation. *Curr. Top. Solution Chem.* **1994**, *1*, 223–239.

(10) Stoppa, A.; Hunger, J.; Buchner, R. Conductivities of Binary Mixtures of Ionic Liquids with Polar Solvents. *J. Chem. Eng. Data* **2009**, *54*, 472–479.

(11) Barthel, J.; Feuerlein, F.; Neueder, R.; Wachter, R. Calibration of Conductance Cells at Various Temperatures. *J. Solution Chem.* **1980**, *9*, 209–219.

(12) Hoover, T. B. Conductance of Potassium Chloride in Highly Purified N-methylpropionamide from 20 to 40°. *J. Phys. Chem.* **1964**, *68*, 876–879.

(13) Casteel, J. F.; Amis, A. S. Specific Conductance of Concentrated Solutions of Magnesium Salts in Water-Ethanol System. *J. Chem. Eng. Data* **1972**, *17* (1), 55–59.

(14) Buchner, R.; Capewell, S. G.; Hefter, G.; May, P. M. Ion-pair and Solvent Relaxation Processes in Aqueous Na_2SO_4 Solutions. *J. Phys. Chem. B* **1999**, *103*, 1185–1192.

(15) Fleming, R. Some Physical Properties of Aqueous Solutions of Choline Chloride at 25 °C. *J. Chem. Soc. A* **1960**, 4914–4916.

(16) Spieweck, F.; Bettin., H. Review: Solid and Liquid Density Determination. *Tech. Messen* **1992**, *59*, 285–292.

(17) Desnoyers, J. E.; Arel, M. Apparent Molal Volumes of n-Alkylamine Hydrobromides in Water at 25 °C: Hydrophobic Hydration and Volume Changes. *Can. J. Chem.* **1967**, *45*, 359–366.

(18) Redlich, O.; Meyer, D. M. The Molal Volumes of Electrolytes. *Chem. Rev.* **1964**, *64* (3), 221–227.

(19) Millero, F. J. The Molal Volumes of Electrolytes. *Chem. Rev.* **1971**, *71* (2), 147–176.

(20) Archer, D. J.; Wang, P. The Dielectric Constant of Water and Debye-Hückel Limiting Law Slopes. *J. Phys. Chem. Ref. Data* **1990**, *19*, 371–411.

(21) Klofutar, C.; Horvat, J.; Rudan-Tasič, D. Apparent Molar Volume and Apparent Molar Expansibility of Sodium Saccharin, Potassium Acesulfame and Aspartame. *Acta Chim. Slov.* **2006**, *53*, 274–283.

(22) Hepler, L. G. Thermal Expansion and Structure in Water and Aqueous Solutions. *Can. J. Chem.* **1969**, *47*, 4613–4617.

(23) Millero, F. J. The Apparent and Partial Molal Volume of Aqueous Sodium Chloride Solutions at Various Temperatures. *J. Phys. Chem.* **1970**, *74* (2), 356–362.

(24) Bešter-Rogač, M.; Neueder, R.; Barthel, J. Conductivity of Sodium Chloride in Water + 1,4-Dioxane Mixtures at Temperatures from 5 to 35 °C. I. Dilute Solutions. *J. Solution Chem.* **1999**, *28*, 1071–1086.

(25) Bockris, J. O'M.; Reddy, A. K. N. *Modern Electrochemistry*, Vol. 1, 2nd ed.; Plenum: New York, 1998.

(26) Apelblat, A. Limiting Conductances of Electrolytes and The Walden Product in Mixed Solvents in a Phenomenological Approach. *J. Phys. Chem. B* **2008**, *112*, 7032–7044.