Supplementary Material for

Thermal Conductivity of Aqueous Solutions of Reline, Ethaline, and Glyceline Deep Eutectic Solvents; A Molecular Dynamics Simulation Study

Alper T. Celebi, Thijs J. H. Vlugt, and Othonas A. Moultos

Engineering Thermodynamics, Process & Energy Department, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Leeghwaterstraat 39, 2628CB Delft, The Netherlands

CONTACT Othonas A. Moultos Email: o.moultos@tudelft.nl

1. Introduction

In the Supplementary Material, force field parameters of all simulated systems are listed. Raw data for computed densities and thermal conductivities of aqueous reline, ethaline, and glyceline solutions are presented as a function of the mass fraction of water and temperature.

2. Force field parameters

2.1. Force field parameters for reline-water mixtures

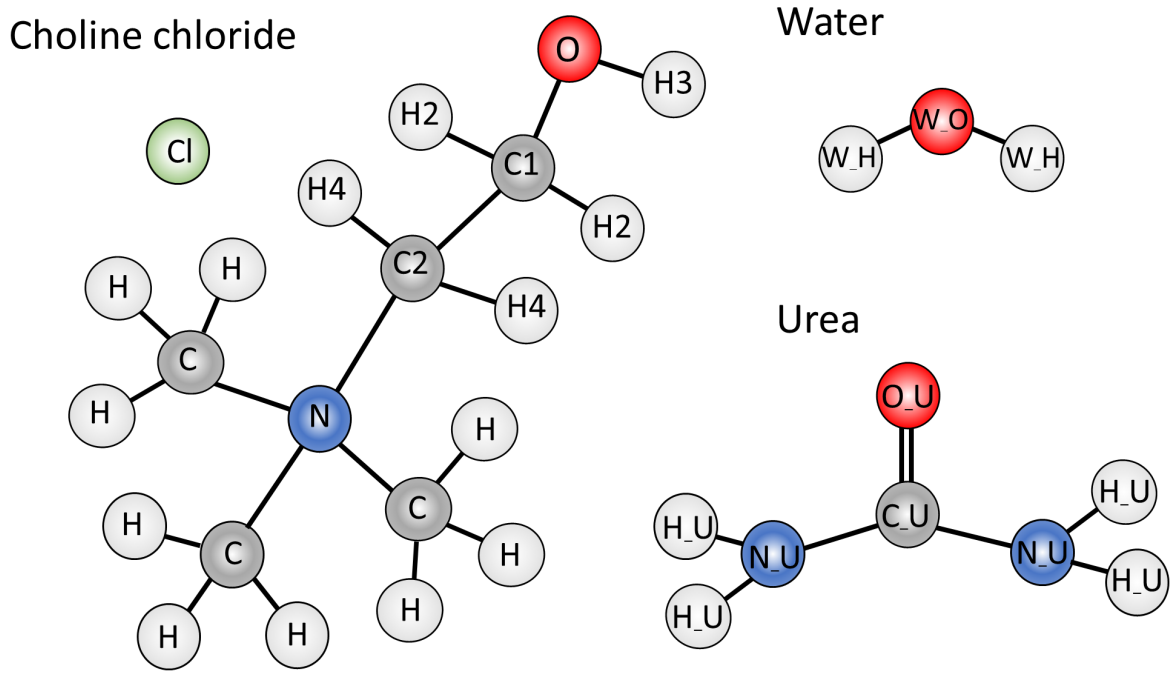

Figure S1: Molecular structure of choline chloirde, urea and water, and atom labels.

Table S1.: Partial charges, masses and Lennard-Jones parameters for all atomic species for choline chloride/urea and water mixtures. Choline chloride and urea parameters are taken by Perkins et al. [1] Water molecules are modeled using the the SPC/E water model [2]. See Figure S1 for the atom labels.

No	Name	$q/[e]$	$m/[\mathrm{u}]$	$\epsilon/k_\mathrm{B}/[\mathrm{K}]$	$\sigma/[\mathrm{Å}]$
1	C	-0.10736	12.0107	55.052	3.3996
2	C1	0.12008	12.0107	55.052	3.3996
3	C2	-0.02576	12.0107	55.052	3.3996
4	C_U	1.0401	12.0107	43.277	3.3996
5	Cl	-0.8	35.453	50.322	4.401
6	H	0.09544	1.00794	7.901	1.9599
7	H2	0.0408	1.00794	7.901	2.4713
8	H3	0.3636	1.00794	0.503	0.1
9	H4	0.08928	1.00794	7.901	1.9599
10	H_U	0.4167	1.00794	7.901	1.069
11	N	0.04016	14.0067	85.547	3.2499
12	N_U	-1.0246	14.0067	85.547	3.25
13	O	-0.49512	15.9994	105.877	3.0664
14	O_U	-0.6577	15.9994	105.676	2.96
15	W_H	0.424	1.00794	0	0
16	W_O	-0.848	15.9994	78.200	3.1656

Table S2.: Bond-stretching parameters for water-reline mixtures. Choline choride and urea molecules are modelled using GAFF [3]. Water molecules are modelled using the the SPC/E model [2]. See Figure S1 for the atom labels. The bond-stretching energy is calculated as: $E_{\mathrm{Bond}}(r)=K_{\mathrm{r}}(r\text{-}r_0)^2$.

No	Name	$K_{\mathrm{r}}/k_{\mathrm{B}}$/[K Å^{-2}]	r_0/[Å]
1	C-H	170440.5	1.09
2	C2-N	147745.3	1.5
3	C1-O	158061.3	1.43
4	C1-H2	169031.5	1.09
5	H_U-N_U	206420.7	1.01
6	C-N	147745.3	1.5
7	C1-C2	152525.9	1.54
8	W_H-W_O	226448.9	1
9	C2-H4	170440.5	1.09
10	C_U-N_U	240639.7	1.35
11	H3-O	185990.0	0.97
12	C_U-O_U	326086.4	1.21

Table S3.: Angle-bending parameters for water-reline mixtures. Choline choride and urea molecules are modelled using GAFF [3]. Water molecules are modelled using the SPC/E model [2]. See Figure S1 for the atom labels. The bond-stretching energy is calculated as: $E_{\mathrm{Angle}}(\theta)=K_\theta(\theta\text{-}\theta_0)^2$.

No	Name	K_θ/k_{B}/[K rad^{-2}]	θ_0
1	C-N-C2	31622.3	110.6
2	H2-C1-H2	19716.1	109.6
3	C2-C1-O	34078.0	109.4
4	H-C-N	24667.8	107.9
5	C2-C1-H2	23329.3	110.1
6	W_H-W_O-W_H	27677.1	109.47
7	C_U-N_U-H_U	24763.4	118.5
8	H2-C1-O	25649.1	109.9
9	C1-O-H3	23696.6	108.2
10	H4-C2-N	24667.8	107.9
11	C1-C2-N	32432.5	114.3
12	H_U-N_U-H_U	19992.9	117.9
13	N_U-C_U-N_U	37640.8	113.4
14	H-C-H	19645.7	110.7
15	N_U-C_U-O_U	38159.1	122
16	C-N-C	31622.3	110.6
17	H4-C2-H4	19645.7	110.7
18	C1-C2-H4	23158.2	111.7

Table S4.: Dihedral torsion parameters for water-reline mixtures. Choline choride and urea molecules are modelled using GAFF [3]. See Figure S1 for the atom labels. The torsion energy for the Charmm style is calculated as: $E_{\mathrm{Dihedral}}(\phi)=\frac{V_n}{2}[1+\cos(n\phi\text{-}\gamma)]$. The torsion energy for the OPLS style is calculated as: $E_{\mathrm{Dihedral}}(\phi)=\frac{K_1}{2}[1+\cos(\phi)]+\frac{K_2}{2}[1\text{-}\cos(2\phi)]+\frac{K_3}{2}[1+\cos(3\phi)]$.

No	Name	$V_{\mathrm{n}}/2/k_{\mathrm{B}}$/[K]	n	γ	Style
1	H4-C2-N-C	78.50	3	0	Charmm
2	C1-C2-N-C	78.50	3	0	Charmm
3	O-C1-C2-H4	78.50	3	0	Charmm
4	H-C-N-C2	78.50	3	0	Charmm
5	H2-C1-C2-H4	78.50	3	0	Charmm
6	N_U-C_U-N_U-H_U	1258.05	2	180	Charmm
7	H2-C1-O-H3	84.04	3	0	Charmm
8	H2-C1-C2-N	78.50	3	0	Charmm
9	H-C-N-C	78.50	3	0	Charmm
10	O-C1-C2-N	78.50	3	0	Charmm
No	Name	K_1/k_{B}/[K]	K_2/k_{B}/[K]	K_3/k_{B}/[K]	Style
11	O_U-C_U-N_U-H_U	2012.88	2516.10	0	OPLS
12	C2-C1-O-H3	251.61	0	161.03	OPLS

Table S5.: Improper torsion parameters for water-reline mixtures. Choline choride and urea molecules are modelled using GAFF [3]. See Figure S1 for the atom labels. The torsion energy is calculated as: $E_{\mathrm{Dihedral}}(\phi)=\frac{V_n}{2}[1+\cos(n\phi\text{-}\gamma)]$.

No	Name	$V_{\mathrm{n}}/2/k_{\mathrm{B}}/[\mathrm{K}]$	n	γ
1	C_U-H_U-N_U-H_U	553.54	180	2
2	N_U-N_U-C_U-O_U	5283.81	180	2

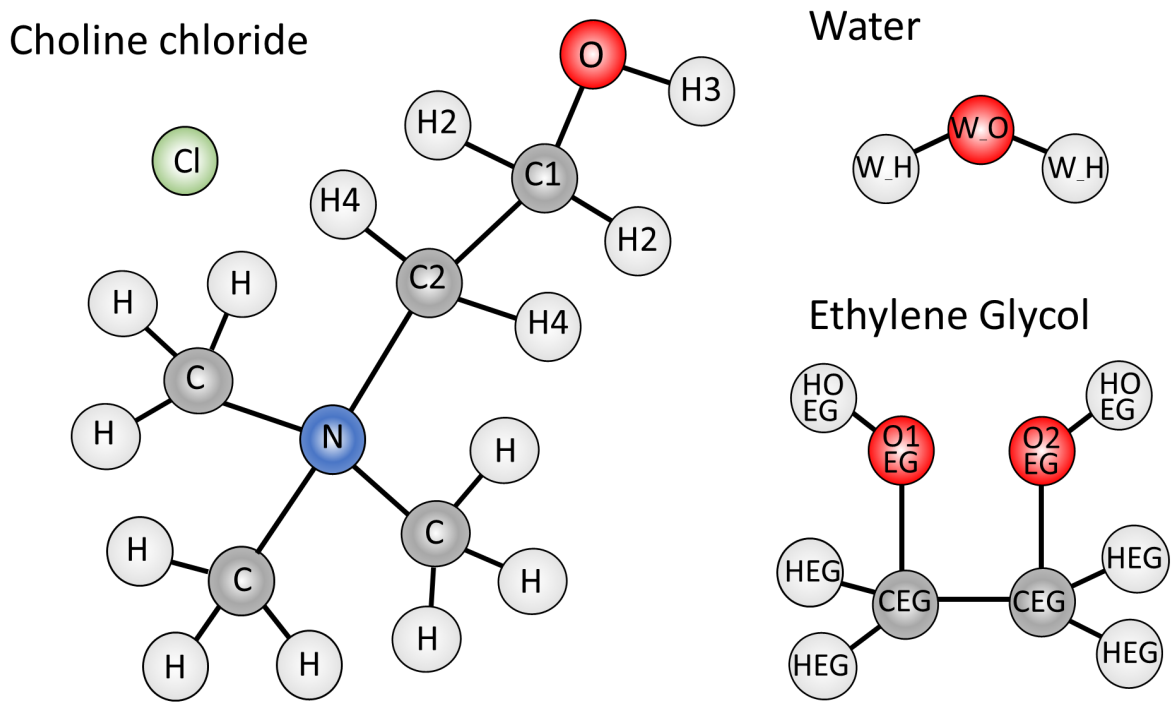

Figure S2: Molecular structure of choline chloirde, ethylene glycol and water, and atom labels.

Table S6.: Partial charges, masses and Lennard-Jones parameters for all atomic species for choline chloride/ethylene glycol and water mixtures. Choline chloride and ethylene glycol parameters are taken by Perkins et al. [1] Water molecules are modeled using the the SPC/E water model [2]. See Figure S1 for the atom labels.

No	Name	$q/[e]$	$m/[\mathrm{u}]$	$\epsilon/k_\mathrm{B}/[\mathrm{K}]$	$\sigma/[\mathrm{Å}]$
1	C	-0.12078	12.0107	55.052	3.3996
2	C1	0.13509	12.0107	55.052	3.3996
3	C2	-0.02898	12.0107	55.052	3.3996
4	CEG	0.1615	12.0107	55.052	3.3996
5	Cl	-0.9	35.453	50.322	4.401
6	H	0.10737	1.00794	7.901	1.9599
7	H2	0.0459	1.00794	7.901	2.4713
8	H3	0.40905	1.00794	0.503	0.1
9	H4	0.10044	1.00794	7.901	1.9599
10	HEG	0.0328	1.00794	7.901	2.4713
11	HOEG	0.4069	1.00794	0.503	0.1
12	N	0.04518	14.0067	85.547	3.2499
13	O	-0.55701	15.9994	105.877	3.0664
14	O1EG	-0.6340	15.9994	105.877	3.0664
15	O2EG	-0.6340	15.9994	105.877	3.0664
16	W_H	0.424	1.00794	0	0
17	W_O	-0.848	15.9994	78.200	3.1656

Table S7.: Bond-stretching parameters for ethaline-water mixtures. Choline choride and ethylene glycol molecules are modelled using GAFF [3]. Water molecules are modelled using the the SPC/E model [2]. See Figure S2 for the atom labels. The bond-stretching energy is calculated as: $E_{\mathrm{Bond}}(r)=K_{\mathrm{r}}(r\text{-}r_0)^2$.

No	Name	$K_{\mathrm{r}}/k_{\mathrm{B}}$/[K Å^{-2}]	r_0/[Å]
1	C-H	170440.5	1.091
2	C2-N	147745.3	1.499
3	C1-O	158061.3	1.426
4	C1-H2	169031.5	1.093
5	CEG-CEG	152525.9	1.535
6	C1-C2	152525.9	1.535
7	C-N	147745.3	1.499
8	W_H-W_O	226448.9	1
9	CEG-HEG	169031.5	1.093
10	CEG-O1EG	158061.3	1.426
11	CEG-O2EG	158061.3	1.426
12	HOEG-O1EG	185990.0	0.974
13	HOEG-O2EG	185990.0	0.974
14	C2-H4	170440.5	1.091
15	H3-O	185990.0	0.974

Table S8.: Angle-bending parameters for water-ethaline mixtures. Choline choride and ethylene glycol molecules are modelled using GAFF [3]. Water molecules are modelled using the the SPC/E model [2]. See Figure S2 for the atom labels. The angle-bending energy is calculated as: $E_{\mathrm{Angle}}(\theta)=K_\theta(\theta\text{-}\theta_0)^2$.

No	Name	K_θ/k_B/[K rad^{-2}]	θ_0
1	CEG-O1EG-HOEG	23701.6	108.16
2	C-N-C2	31602.2	110.64
3	HEG-CEG-O1EG	25664.2	109.88
4	HEG-CEG-O2EG	25664.2	109.88
5	H2-C1-H2	19726.2	109.55
6	C2-C1-O	34068.0	109.43
7	H-C-N	24657.8	107.91
8	CEG-CEG-O1EG	34068.0	109.43
9	CEG-CEG-HEG	23349.4	110.07
10	CEG-CEG-O2EG	34068.0	109.43
11	C2-C1-H2	23349.4	110.07
12	W_H-W_O-W_H	27677.1	109.47
13	H2-C1-O	25664.2	109.88
14	C1-O-H3	23701.6	108.16
15	CEG-O2EG-HOEG	23701.6	108.16
16	HEG-CEG-HEG	19726.2	109.55
17	C1-C2-N	33212.5	108.93
18	H4-C2-N	24657.8	107.91
19	H-C-H	19625.6	110.74
20	C-N-C	31602.2	110.64
21	C1-C2-H4	23148.1	111.74
22	H4-C2-H4	19625.6	110.74

Table S9.: Dihedral torsion parameters for water-ethaline mixtures. Choline choride and ethylene glycol molecules are modelled using GAFF [3]. See Figure S2 for the atom labels. The torsion energy for the Charmm style is calculated as: $E_{\mathrm{Dihedral}}(\phi)=\frac{V_n}{2}[1+\cos(n\phi\text{-}\gamma)]$. The torsion energy for the OPLS style is calculated as: $E_{\mathrm{Dihedral}}(\phi)=\frac{K_1}{2}[1+\cos(\phi)]+\frac{K_2}{2}[1-\cos(2\phi)]+\frac{K_3}{2}[1+\cos(3\phi)]$. The torsion energy for multi/harmonic style is calculated as: $E_{\mathrm{Dihedral}}(\phi)=\sum K_n\cos^{n\,-\,1}(\phi)$.

No	Name	$V_\mathrm{n}/2/k_\mathrm{B}$/[K]	n	γ	Style
1	HEG-CEG-O1EG-HOEG	84.04	3	0	Charmm
2	C1-C2-N-C	78.50	3	0	Charmm
3	H4-C2-N-C	78.50	3	0	Charmm
4	O-C1-C2-H4	78.50	3	0	Charmm
5	HEG-CEG-CEG-HEG	78.50	3	0	Charmm
6	H-C-N-C2	78.50	3	0	Charmm
7	H2-C1-C2-H4	78.50	3	0	Charmm
8	H2-C1-O-H3	84.04	3	0	Charmm
9	H2-C1-C2-N	78.50	3	0	Charmm
10	HEG-CEG-O2EG-HOEG	84.04	3	0	Charmm
11	H-C-N-C	78.50	3	0	Charmm
12	HEG-CEG-CEG-O1EG	125.80	1	0	Charmm
13	O-C1-C2-N	78.50	3	0	Charmm
14	HEG-CEG-CEG-O2EG	125.80	1	0	Charmm

No	Name	K_1/k_B/[K]	K_2/k_B/[K]	K_3/k_B/[K]	Style
15	CEG-CEG-O2EG-HOEG	251.61	0	161.03	OPLS
16	C2-C1-O-H3	251.61	0	161.03	OPLS
17	CEG-CEG-O1EG-HOEG	251.61	0	161.03	OPLS

No	Name	K_1/k_B/[K]	K_2/k_B/[K]	K_3/k_B/[K]	Style
18	O1EG-CEG-CEG-O2EG	72.46	-217.39	1182.57	multi/harmonic
		K_4/k_B/[K]	K_5/k_B/[K]		
		289.85	0		

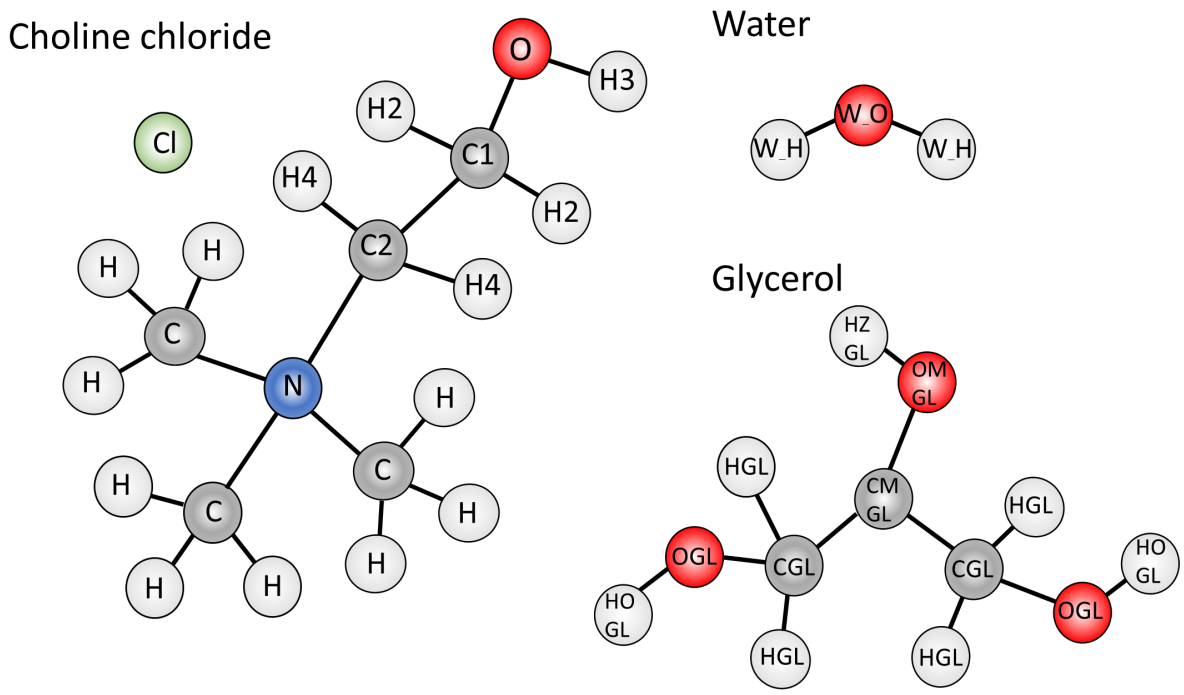

Figure S3: Molecular structure of choline chloirde, glycerol and water, and atom labels.

Table S10.: Partial charges, masses and Lennard-Jones parameters for all atomic species for choline chloride/glycerol and water mixtures. Choline chloride and glycerol parameters are taken by Perkins et al. [1] Water molecules are modeled using the the SPC/E water model [2]. See Figure S1 for the atom labels.

No	Name	$q/[e]$	$m/[\mathrm{u}]$	$\epsilon/k_\mathrm{B}/[\mathrm{K}]$	$\sigma/[\mathrm{Å}]$
1	C	-0.12078	12.0107	55.052	3.3996
2	C1	0.13509	12.0107	55.052	3.3996
3	C2	-0.02898	12.0107	55.052	3.3996
4	CGL	0.1197	12.0107	55.052	3.3996
5	CML	0.152	12.0107	55.052	3.3996
6	Cl	-0.9	35.453	50.322	4.401
7	H	0.10737	1.00794	7.901	1.9599
8	H2	0.0459	1.00794	7.901	2.4713
9	H3	0.40905	1.00794	0.503	0.1
10	H4	0.10044	1.00794	7.901	1.9599
11	HGL	0.0537	1.00794	7.901	2.4713
12	HMGL	0.3912	1.00794	0.503	0.1
13	HOGL	0.4096	1.00794	0.503	0.1
14	HZGL	0.0221	1.00794	7.901	2.4713
15	N	0.04518	14.0067	85.547	3.2499
16	O	-0.55701	15.9994	105.877	3.0664
17	OGL	-0.627	15.9994	105.877	3.0664
18	OMGL	-0.5848	15.9994	105.877	3.0664
19	W_H	0.424	1.00794	0	0
20	W_O	-0.848	15.9994	78.200	3.1656

Table S11.: Bond-stretching parameters for glyceline-water mixtures. Choline choride and glycerol molecules are modelled using GAFF [3]. Water molecules are modelled using the the SPC/E model [2]. See Figure S3 for the atom labels. The bond-stretching energy is calculated as: $E_{\mathrm{Bond}}(r)=K_{\mathrm{r}}(r\text{-}r_0)^2$.

No	Name	$K_{\mathrm{r}}/k_{\mathrm{B}}$/[K Å^{-2}]	r_0/[Å]
1	C-H	170440.5	1.091
2	C2-N	147745.3	1.499
3	C1-O	158061.3	1.426
4	HOGL-OGL	185990.0	0.974
5	C1-H2	169031.5	1.093
6	CMGL-HZGL	169031.5	1.093
7	C-N	147745.3	1.499
8	C1-C2	152525.9	1.535
9	CGL-HGL	169031.5	1.093
10	CMGL-OMGL	158061.3	1.426
11	W_H-W_O	226448.9	1
12	HMGL-OMGL	185990.0	0.974
13	CGL-OGL	158061.3	1.426
14	C2-H4	170440.5	1.091
15	CGL-CMGL	152525.9	1.535
16	H3-O	185990.0	0.974

Table S12.: Angle-bending parameters for water-glyceline mixtures. Choline choride and glycerol molecules are modelled using GAFF [3]. Water molecules are modelled using the the SPC/E model [2]. See Figure S3 for the atom labels. The angle-bending energy is calculated as: $E_{\mathrm{Angle}}(\theta)=K_\theta(\theta\text{-}\theta_0)^2$.

No	Name	K_θ/k_{B}/[K rad^{-2}]	θ_0
1	C-N-C2	31602.2	110.64
1	CGL-CMGL-CGL	31804.2	110.64
3	H2-C1-H2	19726.2	109.55
4	C2-C1-O	34068.0	109.43
5	H-C-N	24657.8	107.91
6	CGL-OGL-HOGL	23701.6	108.16
7	CMGL-CGL-OGL	34068.0	109.43
8	CMGL-CGL-OGL	25664.2	109.88
9	C2-C1-H2	23349.4	110.07
10	W_H-W_O-W_H	27677.1	109.47
11	H2-C1-O	25664.2	109.88
12	CGL-CMGL-HZGL	23349.4	110.07
13	C1-O-H3	23701.6	108.16
14	CMGL-CGL-OGL	25664.2	109.88
15	H4-C2-N	24657.8	107.91
16	C1-C2-N	33212.5	108.93
17	CGL-CMGL-OMGL	34068.0	109.43
18	CMGL-OMGL-HMGL	23701.6	108.16
19	H-C-H	19625.6	110.74
20	CMGL-CGL-HGL	23349.4	110.07
21	HGL-CGL-HGL	19726.2	109.55
22	C-N-C	31602.2	110.64
23	H4-C2-H4	19625.6	110.74
24	C1-C2-H4	23148.1	111.74

Table S13.: Dihedral torsion parameters for water-glyceline mixtures. Choline choride and glycerol molecules are modelled using GAFF [3]. See Figure S3 for the atom labels. The torsion energy for the Charmm style is calculated as: $E_{\mathrm{Dihedral}}(\phi)=\frac{V_n}{2}[1+\cos(n\phi\text{-}\gamma)]$. The torsion energy for the OPLS style is calculated as: $E_{\mathrm{Dihedral}}(\phi)=\frac{K_1}{2}[1+\cos(\phi)]+\frac{K_2}{2}[1\text{-}\cos(2\phi)]+\frac{K_3}{2}[1+\cos(3\phi)]$. The torsion energy for multi/harmonic style is calculated as: $E_{\mathrm{Dihedral}}(\phi)=\sum K_n\cos^{n\text{ - }1}(\phi)$.

No	Name	$V_\mathrm{n}/2/k_\mathrm{B}$/[K]	n	γ	Style
1	HGL-CGL-CMGL-HZGL	78.50	3	0	Charmm
2	H4-C2-N-C	78.50	3	0	Charmm
3	C1-C2-N-C	78.50	3	0	Charmm
4	HGL-CGL-CMGL-OMGL	125.80	1	0	Charmm
5	O-C1-C2-H4	78.50	3	0	Charmm
6	H-C-N-C2	78.50	3	0	Charmm
7	H2-C1-C2-H4	78.50	3	0	Charmm
9	OGL-CGL-CMGL-HZGL	125.80	1	0	Charmm
10	H2-C1-O-H3	84.04	3	0	Charmm
11	OGL-CGL-CMGL-CGL	78.50	3	0	Charmm
12	H2-C1-C2-N	78.50	3	0	Charmm
13	HGL-CGL-CMGL-CGL	78.50	3	0	Charmm
16	H-C-N-C	78.50	3	0	Charmm
17	HGL-CGL-OGL-HOGL	84.04	3	0	Charmm
19	O-C1-C2-N	78.50	3	0	Charmm
20	HZGL-CMGL-OMGL-HMGL	84.04	3	0	Charmm

No	Name	K_1/k_B/[K]	K_2/k_B/[K]	K_3/k_B/[K]	Style
8	CGL-CMGL-OMGL-HMGL	251.61	0	161.03	OPLS
15	C2-C1-O-H3L	251.61	0	161.03	OPLS
18	CMGL-CGL-OGL-HOGL	251.61	0	161.03	OPLS

No	Name	K_1/k_B/[K]	K_2/k_B/[K]	K_3/k_B/[K]	Style
14	OGL-CGL-CMGL-OMGL	72.46	-217.39	1182.57	multi/harmonic
		K_4/k_B/[K]	K_5/k_B/[K]		
		289.85	0		

3. Results

Table S14.: The number of molecules for aqueous reline, ethaline and glyceline solutions at 303.15 K and 1 atm. The number of molecules for each system were specifically determined to make the final box size of each system 5.5 nm.

Water Mass Fraction/[%]	**Reline Mixtures**			
	Number of Molecules			**Box Size/[nm]**
	Urea	**ChCl**	**Water**	
0	936	468	0	5.5
25	672	336	1615	5.5
50	426	213	3071	5.5
75	202	101	4368	5.5
100	0	0	5534	5.5
Water Mass Fraction/[%]	**Ethaline Mixtures**			
	Number of Molecules			**Box Size/[nm]**
	EG	**ChCl**	**Water**	
0	850	425	0	5.5
25	628	314	1532	5.5
50	406	203	2972	5.5
75	196	98	4304	5.5
100	0	0	5534	5.5
Water Mass Fraction/[%]	**Glyceline Mixtures**			
	Number of Molecules			**Box Size/[nm]**
	Glycerol	**ChCl**	**Water**	
0	768	369	0	5.5
25	534	267	1600	5.5
50	340	170	3055	5.5
75	162	81	4368	5.5
100	0	0	5534	5.5

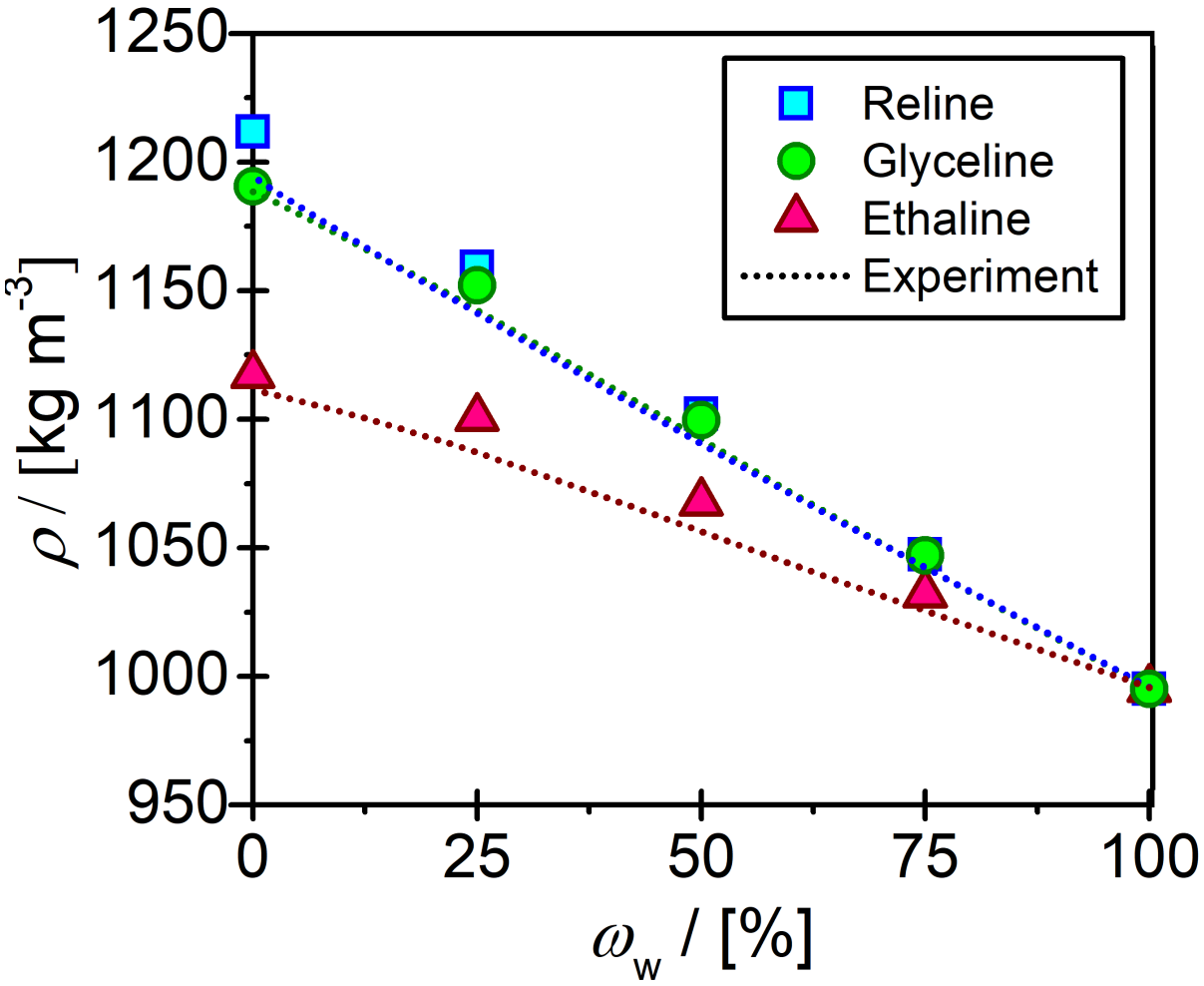

Figure S4: Densities of aqueous reline, ethaline, and glyceline solutions at 303.15 K and 1 atm as a function of the mass fraction of water. MD results are compared to experimental data by Yadav et al. [4–6]

Table S15.: Average densities of aqueous reline, ethaline and glyceline solutions as a function of the mass fraction of water at 303.15 K and 1 atm. MD results are compared with experimental values by Yadav et al.[4–6]

Computed Densities/[kg m^{-3}]					
T=303.15K	**Water Mass Fraction/[%]**				
	0	**25**	**50**	**75**	**100**
Reline	1211.7	1159.2	1102.1	1047.4	995.2
Ethaline	1117.3	1100.5	1067.7	1032.0	995.2
Glyceline	1190.6	1152.1	1099.7	1047.0	995.2
Experimental Densities/[kg m^{-3}]					
T=303.15K	**Water Mass Fraction/[%]**				
	0	**25**	**50**	**75**	**100**
Reline	1194.5	1140.8	1090.4	1042.3	995.4
Ethaline	1111.4	1087.0	1056.6	1024.6	995.4
Glyceline	1188.5	1142.4	1092.2	1042.1	995.4

Table S16.: The number of Argon atoms and reline molecules for various system sizes. The density of liquid argon at 86 K and 1 atm is 1403 kg/m^3), and the density of neat reline at 303.15 K and 1 atm is 1212 kg/m^3).

L_{Argon} / [nm]	$\#_{\text{Argon}}$	L_{Reline} / [nm]	$\#_{\text{Reline}}$
2.17	216	2.63	51
2.53	343	3.01	77
2.89	512	3.31	102
3.25	729	3.81	155
3.62	1000	4.17	204
4.70	2197	5.26	408
5.83	4196	6.02	612
7.23	8000	7.14	1023
9.04	15625	8.25	1575
9.76	19683		
10.8	27000		
11.9	35937		
13.4	50653		
14.5	64000		
20.2	175616		
24.9	328509		
30.0	571787		

Table S17.: Computed thermal conductivities of aqueous reline, ethaline and glyceline solutions as a function of the mass fraction of water at 303.15 K and 1 atm.

Thermal Conductivities/[W $m^{-1}K^{-1}$]					
	Water Mass Fraction/[%]				
	0	**25**	**50**	**75**	**100**
Reline	0.244±0.005	0.460±0.006	0.596±0.005	0.738±0.009	0.853±0.008
Ethaline	0.228±0.005	0.386±0.005	0.528±0.004	0.695±0.003	0.853±0.008
Glyceline	0.237±0.003	0.417±0.005	0.558±0.006	0.715±0.006	0.853±0.008

Table S18.: Influence of the temperature on the computed thermal conductivity of neat and aqueous glyceline solutions.

Thermal Conductivities/[W $m^{-1}K^{-1}$]					
	Temperature/[K]				
	283.15	**303.15**	**323.15**	**343.15**	**363.15**
Neat Glyceline	0.236±0.003	0.237±0.005	0.239±0.006	0.243±0.006	0.247±0.005
Aq. Glyceline (25%)	0.412±0.006	0.417±0.005	0.411±0.004	0.422±0.006	0.425±0.003
Aq. Glyceline (50%)	0.551±0.005	0.557±0.005	0.556±0.005	0.566±0.006	0.561±0.004
Aq. Glyceline (75%)	0.719±0.009	0.704±0.005	0.715±0.008	0.726±0.007	0.716±0.008
Water	0.848±0.007	0.858±0.007	0.863±0.002	0.863±0.002	0.858±0.001

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