Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Janus-Faced Role of Water in Defining Nanostructure of Choline Chloride/Glycerol Deep Eutectic Solvent

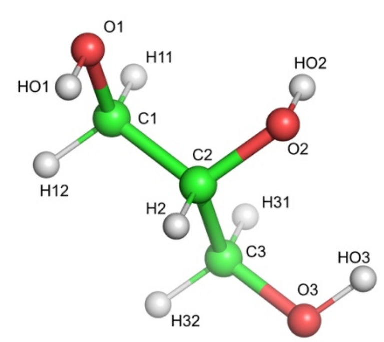
Lindong Weng and Mehmet Toner

Supplementary information

Table S1. Atom type and partial charge of glycerol[a] and choline[b]

Glycerol			Choline		
Atom ID	Atom Type	Charge	Atom ID	Atom Type	Charge
C1	C321	0.05	N	N3P0	-0.60
C2	C311	0.14	C1	C321	0.05
C3	C321	0.05	H11	HGA2	0.09
O1	O311	-0.65	H12	HGA2	0.09
H11	HGA2	0.09	OC1	O311	-0.65
H12	HGA2	0.09	HO1	HGP1	0.42
O2	O311	-0.65	C2	C324	-0.10
H2	HGA1	0.09	H21	HGP5	0.25
O3	O311	-0.65	H22	HGP5	0.25
H32	HGA2	0.09	C3	C334	-0.35
H31	HGA2	0.09	H31	HGP5	0.25
HO1	HGP1	0.42	H32	HGP5	0.25
HO2	HGP1	0.42	H33	HGP5	0.25
HO3	HGP1	0.42	C4	C334	-0.35
			H41	HGP5	0.25
			H42	HGP5	0.25
			H43	HGP5	0.25
			C5	C334	-0.35
			H51	HGP5	0.25
			H52	HGP5	0.25
			H53	HGP5	0.25

a



b

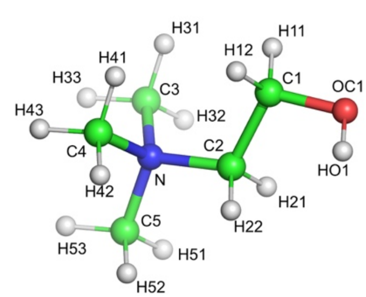


Table S2. Parameters for bond, angle, dihedral and non-bonded interactions of glycerol[a]

Bond			
		K_b (kcal/mol/Å^2)	b_0 (Å)
C311	C321	222.5	1.538
C321	O311	428.0	1.420
C321	HGA2	309.0	1.111
C311	O311	428.0	1.420
C311	HGA1	309.0	1.111
HGP1	O311	545.0	0.960

Angle				
			K_θ (kcal/mol/rad^2)	θ_0 (°)
C321	C311	C321	58.35	113.5
O311	C311	C321	75.70	110.0
HGA1	C311	C321	34.50	110.1
C311	C321	O311	75.70	110.1
C311	C321	HGA2	33.43	110.1
HGA2	C321	O311	45.90	108.9
C321	O311	HGP1	50.00	106.0
HGA2	C321	HGA2	35.50	109.0
HGA1	C311	O311	45.90	108.9
C311	O311	HGP1	50.00	106.0

Dihedral						
				k (kcal/mol)	n	φ (°)
O311	C321	C311	C321	0.200	3	180
HGA2	C321	C311	C321	0.195	1	0
HGP1	O311	C311	C321	0.300	3	0
HGP1	O311	C311	C321	0.300	1	0
O311	C311	C321	O311	0.200	3	0
O311	C311	C321	HGA2	0.195	3	180
HGA1	C311	C321	O311	0.195	3	0
HGA1	C311	C321	HGA2	0.195	3	0
C311	C321	O311	HGP1	0.140	2	0
C311	C321	O311	HGP1	0.240	3	0
C311	C321	O311	HGP1	1.130	1	0
HGA2	C321	O311	HGP1	0.000	3	0
HGA1	C311	O311	HGP1	0.000	3	0

Non-bonded		
	ε (kcal/mol)	$r_{min}/2$ (Å)
C311	-0.0320	2.0000
C321	-0.0560	2.0100
O311	-0.1921	1.7650
HGA2	-0.0350	1.3400
HGA1	-0.0450	1.3400
HGP1	-0.0460	0.2245

[a] Parameters are organized in the CHARMM format. Physical interpretation of the parameters and their associated equations can be found in the NAMD User's Guide at http://www.ks.uiuc.edu/Research/namd/2.12/ug/.

Table S3. Parameters for bond, angle, dihedral and non-bonded interactions of choline[a]

Bond			
		K_b (kcal/mol/Å^2)	b_0 (Å)
C324	N3P0	215.0	1.510
C334	N3P0	215.0	1.510
C321	HGA2	309.0	1.111
C321	O311	428.0	1.420
C321	C324	222.5	1.530
HGP1	O311	545.0	0.960
C324	HGP5	300.0	1.080
C334	HGP5	300.0	1.080

Angle				
			K_θ (kcal/mol/rad^2)	θ_0 (°)
C321	C324	N3P0	67.70	115.0
HGP5	C324	N3P0	40.00	109.5
C324	N3P0	C334	60.00	109.5
HGP5	C334	N3P0	40.00	109.5
C334	N3P0	C334	60.00	109.5
HGA2	C321	HGA2	35.50	109.0
O311	C321	HGA2	45.90	108.9
C324	C321	HGA2	26.50	110.1
C324	C321	O311	75.70	112.1
C321	O311	HGP1	50.00	106.0
C321	C324	HGP5	33.43	110.1
HGP5	C324	HGP5	24.00	109.5
HGP5	C334	HGP5	24.00	109.5

Dihedral						
				k (kcal/mol)	n	φ (°)
HGA2	C321	C324	N3P0	0.195	3	0
O311	C321	C324	N3P0	4.300	1	180
C321	C324	N3P0	C334	0.260	3	0
HGP5	C324	N3P0	C334	0.260	3	0
C324	N3P0	C334	HGP5	0.260	3	0
HGP5	C334	N3P0	C334	0.260	3	0
HGP1	O311	C321	HGA2	0.000	3	0
HGP5	C324	C321	HGA2	0.195	3	0
HGP5	C324	C321	O311	0.195	3	0
C324	C321	O311	HGP1	0.140	2	0
C324	C321	O311	HGP1	0.240	3	0
C324	C321	O311	HGP1	1.130	1	0

Non-bonded		
	ε (kcal/mol)	$r_{min}/2$ (Å)
C324	-0.0550	2.1750
N3P0	-0.2000	1.8500
C334	-0.0770	2.2150
C321	-0.0560	2.0100
HGA2	-0.0350	1.3400
O311	-0.1921	1.7650
HGP1	-0.0460	0.2245
HGP5	-0.0460	0.7000

[a] Parameters are organized in the CHARMM format. Physical interpretation of the parameters and their associated equations can be found in the NAMD User's Guide at http://www.ks.uiuc.edu/Research/namd/2.12/ug/.