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

Supplementary material

Shah et al: Intermolecular interactions and solvation effects of Dimethylsulfoxide on type III deep eutectic solvents

Table S1: LJ, partial charges, and bond parameters for urea, choline ion, and DMSO molecules. The atom numbers are mentioned in the figure above. All units are standard units used in gromacs.

Urea

Atom No.	Type	Partial Charge	C6	C12
1	HC	0.426	8.46E-05	1.51E-08
2	NT	-0.981	0.00243641	5.06E-06
3	HC	0.426	8.46E-05	1.51E-08
4	C	0.915	0.002340624	4.94E-06
5	O	-0.657	0.002261954	1.00E-06
6	NT	-0.981	0.00243641	5.06E-06
7	HC	0.426	8.46E-05	1.51E-08
8	HC	0.426	8.46E-05	1.51E-08
Bonds				
Atom No.	**Atom No.**	**Function type**	**Bond length**	**Bond constant**
1	2	2	0.101	2.11E+07
2	3	2	0.101	2.11E+07
2	4	2	0.138	1.10E+07
4	5	2	0.123	1.66E+07
4	6	2	0.138	1.10E+07
6	7	2	0.101	2.11E+07
6	8	2	0.101	2.11E+07
Angles				
Atom No.	**Atom No.**	**Atom No.**	**Func.**	**Angle**	**Angle constant**
1	2	3	2	113	545
1	2	4	2	115	460
3	2	4	2	115	460
2	4	5	2	124	730
2	4	6	2	120	560

5	4	6	2	124	730		
4	6	7	2	115	460		
4	6	8	2	115	460		
7	6	8	2	113	545		
Improper Dihedrals							
Atom No.	**Atom No.**	**Atom No.**	**Atom No.**	**Func.**	**Angle**	**Fc**	
4	2	6	5	2	0	167.36	
Proper Dihedrals							
Atom No.	**Atom No.**	**Atom No.**	**Atom No.**	**Func.**	**Phi**	**cp**	**Mult**
1	2	4	5	1	180	5.86	2
5	4	6	8	1	180	5.86	2

Choline ion

Atom No.	Type	Partial Charge	C6	C12
1	HS14	0.442	0	0
2	OA	-0.653	0.002261954	1.51E-06
3	C	0.276	0.002340624	4.94E-06
4	HC	0.029	8.46E-05	1.51E-08
5	HC	0.029	8.46E-05	1.51E-08
6	C	-0.224	0.002340624	4.94E-06
7	HC	0.151	8.46E-05	1.51E-08
8	HC	0.151	8.46E-05	1.51E-08
9	NL	0.346	0.00243641	2.32E-06
10	C	-0.452	0.002340624	4.94E-06
11	HC	0.201	8.46E-05	1.51E-08
12	HC	0.201	8.46E-05	1.51E-08
13	HC	0.201	8.46E-05	1.51E-08
14	C	-0.452	0.002340624	4.94E-06
15	HC	0.201	8.46E-05	1.51E-08
16	HC	0.201	8.46E-05	1.51E-08
17	HC	0.201	8.46E-05	1.51E-08
18	C	-0.452	0.002340624	4.94E-06
19	HC	0.201	8.46E-05	1.51E-08
20	HC	0.201	8.46E-05	1.51E-08
21	HC	0.201	8.46E-05	1.51E-08
Bonds				
Atom No.	**Atom No.**	**Function type**	**Bond length**	**Bond constant**
1	2	2	0.0972	1.96E+07
2	3	2	0.142	3.22E+06
3	4	2	0.109	1.23E+07
3	5	2	0.109	1.23E+07
3	6	2	0.152	5.43E+06
6	7	2	0.109	1.23E+07
6	8	2	0.109	1.23E+07
6	9	2	0.153	7.15E+06
9	10	2	0.151	3.73E+06

9	14	2	0.151		3.73E+06
9	18	2	0.151		3.73E+06
10	11	2	0.109		1.23E+07
10	12	2	0.109		1.23E+07
10	13	2	0.109		1.23E+07
14	15	2	0.109		1.23E+07
14	16	2	0.109		1.23E+07
14	17	2	0.109		1.23E+07
18	19	2	0.109		1.23E+07
18	20	2	0.109		1.23E+07
18	21	2	0.109		1.23E+07
Angles					
Atom No.	**Atom No.**	**Atom No.**	**Func.**	**Angle**	**Angle constant**
1	2	3	2	109.5	450
2	3	4	2	111.4	532
2	3	5	2	111.4	532
2	3	6	2	109.5	520
4	3	5	2	106.75	503
4	3	6	2	111.4	532
5	3	6	2	111.4	532
3	6	7	2	110.3	524
3	6	8	2	110.3	524
3	6	9	2	115	610
7	6	8	2	108.53	443
7	6	9	2	106	1733.55
8	6	9	2	106	1733.55
6	9	10	2	116	620
6	9	14	2	116	620
6	9	18	2	116	620
10	9	14	2	109	1680.51
10	9	18	2	109	1680.51
14	9	18	2	109	1680.51
9	10	11	2	108.53	443
9	10	12	2	108.53	443
9	10	13	2	108.53	443

11	10	12	2	111.3	632
11	10	13	2	111.3	632
12	10	13	2	111.3	632
9	14	15	2	108.53	443
9	14	16	2	108.53	443
9	14	17	2	108.53	443
15	14	16	2	111.3	632
15	14	17	2	111.3	632
16	14	17	2	111.3	632
9	18	19	2	108.53	443
9	18	20	2	108.53	443
9	18	21	2	108.53	443
19	18	20	2	111.3	632
19	18	21	2	111.3	632
20	18	21	2	111.3	632

Proper Dihedrals

Atom No.	Atom No.	Atom No.	Atom No.	Func.	Phi	cp	Mult
1	2	3	6	1	0	1.26	3
2	3	6	9	1	0	5.92	3
3	6	9	18	1	0	1.05	3
6	9	10	11	1	0	1.05	3
6	9	14	15	1	0	1.05	3
6	9	18	19	1	0	1.05	3

DMSO

Atom No.	Type	Partial Charge	C6	C12
1	HDM	0.09	7.44E-05	1.38E-08
2	CDM	-0.148	0.003011	6.94E-06
3	HDM	0.09	7.44E-05	1.38E-08
4	HDM	0.09	7.44E-05	1.38E-08
5	SDM	0.312	0.011996	2.46E-05
6	ODM	-0.556	0.001551	1.20E-06
7	CDM	-0.148	0.003011	6.94E-06
8	HDM	0.09	7.44E-05	1.38E-08

9	HDM	0.09	7.44E-05	1.38E-08
10	HDM	0.09	7.44E-05	1.38E-08

Bonds

Atom No.	Atom No.	Function type	Bond length	Bond constant
1	2	1	0.111	1.35E+05
2	3	1	0.111	1.35E+05
2	4	1	0.111	1.35E+05
2	5	1	0.18	1.00E+05
5	6	1	0.153	2.26E+05
5	7	1	0.18	1.00E+05
7	8	1	0.111	1.35E+05
7	9	1	0.111	1.35E+05
7	10	1	0.111	1.35E+05

Angles

Atom No.	Atom No.	Atom No.	Func.	Angle	Angle constant
1	2	3	1	108.4	148.53
1	2	4	1	108.4	148.53
1	2	5	1	111.3	192.88
3	2	4	1	108.4	148.53
3	2	5	1	111.3	192.88
4	2	5	1	111.3	192.88
2	5	6	1	106.75	330.54
2	5	7	1	95	142.26
6	5	7	1	106.75	330.54
5	7	8	1	111.3	192.88
5	7	9	1	111.3	192.88
5	7	10	1	111.3	192.88
8	7	9	1	108.4	148.53
8	7	10	1	108.4	148.53
9	7	10	1	108.4	148.53

Proper Dihedrals

Atom No.	Atom No.	Atom No.	Atom No.	Func.	Phi	cp	Mult
3	2	5	6	1	0	0.84	3
2	5	7	8	1	0	0.84	3

Table S2. The number of H-bonds between the components according to DMSO and DES concentration.

Components	Urea-Urea	Urea-CHT	Urea-CL	Urea-DMSO	CHT-CL	CHT-DMSO	CL-DMSO	CL-CL	CHT-CHT
Pure DES	158.97	150.19	19.48		194.90			0.00	16.09
0.95 DES - 0.05 DMSO	170.51	165.47	15.97	7.27	181.40	3.12	0.00	0.00	23.51
0.9 DES - 0.1 DMSO	176.56	155.99	15.17	13.77	189.85	4.51	0.00	0.00	18.48
0.7 DES - 0.3 DMSO	165.91	147.18	14.24	44.00	191.51	17.28	0.01	0.00	17.39
0.5 DES - 0.5 DMSO	141.68	136.35	14.63	75.32	179.45	33.85	0.02	0.00	20.69
0.3 DES - 0.7 DMSO	117.83	120.63	13.23	129.70	190.89	61.90	0.02	0.00	14.71
0.1 DES - 0.9 DMSO	71.35	79.98	11.13	256.09	167.67	144.43	0.04	0.00	9.41
Pure DMSO									

Table S3. Diffusion coefficients of the molecules in reline-water mixture. All units are in cm^2/s.

Components	Water mole fraction						
	0.0 (Pure reline)	0.1	0.3	0.5	0.7	0.9	1.0 (Pure water)
Urea	4.37×10^{-8}	5.26×10^{-8}	9.96×10^{-8}	1.00×10^{-7}	2.91×10^{-7}	2.05×10^{-6}	
Choline	3.34×10^{-8}	4.16×10^{-8}	5.59×10^{-8}	7.11×10^{-8}	1.64×10^{-7}	1.17×10^{-6}	
Chloride	2.28×10^{-8}	2.40×10^{-8}	6.20×10^{-8}	6.94×10^{-8}	2.03×10^{-7}	1.83×10^{-6}	
Water		5.90×10^{-8}	1.32×10^{-7}	1.71×10^{-7}	4.14×10^{-7}	3.56×10^{-6}	2.53×10^{-5}
System	3.67×10^{-8}	4.44×10^{-8}	7.85×10^{-8}	9.01×10^{-8}	2.54×10^{-7}	2.40×10^{-6}	