Electronic Supplementary Material (ESI) for Green Chemistry.

Understanding the Role of Co-solvents in the Dissolution of Cellulose in Ionic Liquids

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Electronic Supplementary Information

Contents:

S1: Video of 4 examples of the cellulose dissolution experiments realized with the microscope.

The resolution of the images taken by the microscope has been reduced and the video has been compress to decrease substantially the size of the files.

a) Dissolution 10wt% of cellulose at 50˚C in $[C_4C_1Im][OAc]$.

b) Dissolution of 10wt% of cellulose in $[C_4C_1Im][OAc]$ from 30˚C with a ramp of 1˚C/min.

c) Dissolution of 25wt% of cellulose in $[C_4C_1Im][OAc]$ from 30˚C with a ramp of 0.01˚C/min.

d) Dissolution of 10wt% of cellulose in $[C_4C_1Im][OAc]$/DMSO (x_{IL}=0.25) from 30˚C with a ramp of 1˚C/min.

S2. Conductivity ($mS.cm^{-1}$)

Temperature (˚C)	x_{DMSO}=0.00	x_{DMSO}=0.25	x_{DMSO}=0.50	x_{DMSO}=0.75	x_{DMSO}=1.00
25.00	0.803	1.687	0.3.203	6.350	0.000
30.00	1.108	2.192	0.3.953	7.349	0.005
40.00	1.962	3.503	0.5.753	9.598	0.006
50.00	3.213	5.273	0.8.016	12.214	0.007
60.00	4.937	7.537	10.744	15.195	0.008
80.00	9.939	13.569	17.411	21.937	0.011
100.00	7.026	21.599	25.757	29.468	0.014

VFT fit:
$f(x) = a * \exp (b / (x-t_0))$ with t_0 in Kelvins.

	a	b	t_0
x_{DMSO}=0.00	1334.35	-790.2	191.8
x_{DMSO}=0.25	1228.40	-781.8	179.5
x_{DMSO}=0.50	954.91	-740.3	168.1
x_{DMSO}=0.75	592.77	-663.0	152.0

S3. Viscosity (mPa.s)

Temperature (˚C)	x_{DMSO}=0.00	x_{DMSO}=0.25	x_{DMSO}=0.50	x_{DMSO}=0.75	x_{DMSO}=1.00
25.00	311	118.0	42.6	10.45	1.973
30.00	220	88.7	34.0	8.90	1.795
40.00	117.4	52.5	22.3	6.63	1.504
50.00	69.4	33.8	15.8	5.14	1.285
60.00	43.8	23.1	11.53	4.09	1.118
80.00	21.0	12.3	6.83	2.780	0.874
100.00	11.5	7.60	4.40	2.032	0.713

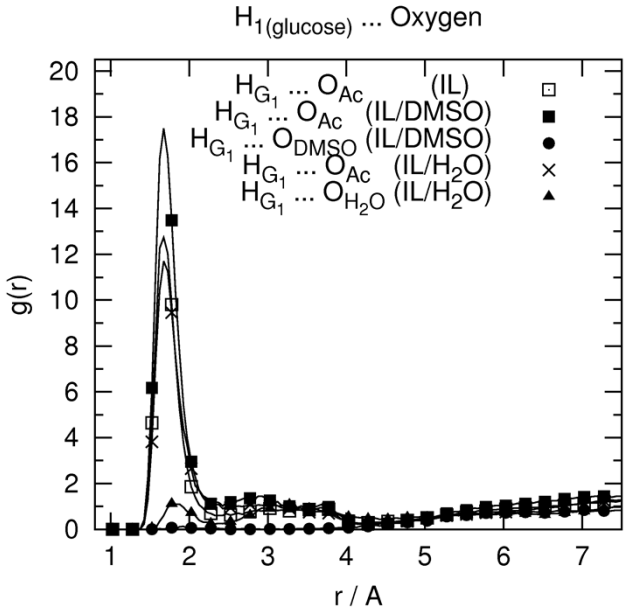
VFT fit:
$f(x) = a * \exp (b / (x-t_0))$ with t_0 in Kelvins.

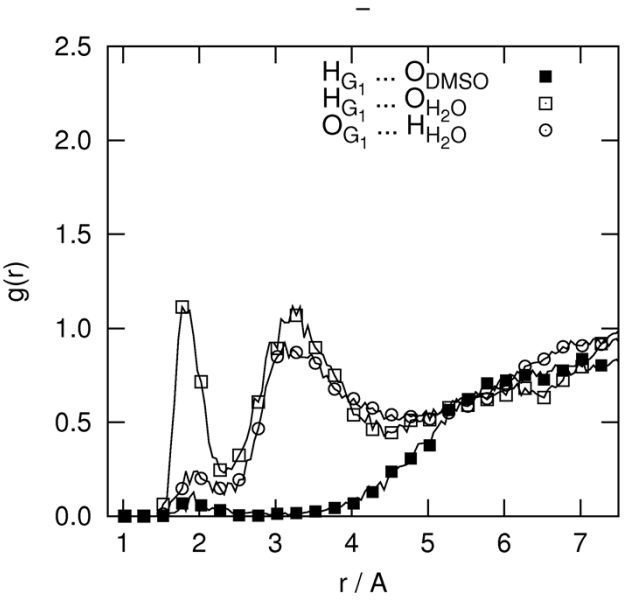
	a	b	t_0
x_{DMSO}=0.00	0.0747	949.76	184.04
x_{DMSO}=0.25	0.1064	808.72	182.67
x_{DMSO}=0.50	0.0894	800.07	168.30
x_{DMSO}=0.75	0.0944	661.85	157.38
x_{DMSO}=1.00	0.0747	543.72	131.9

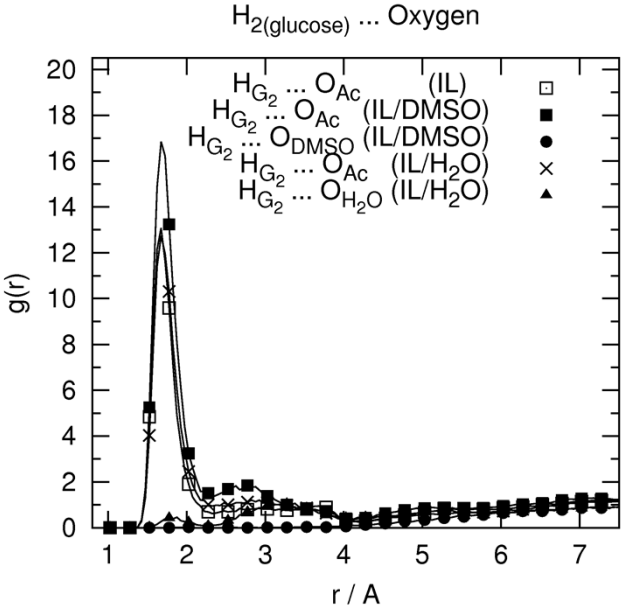
S4. Number of molecules or ion pairs for each simulation box.

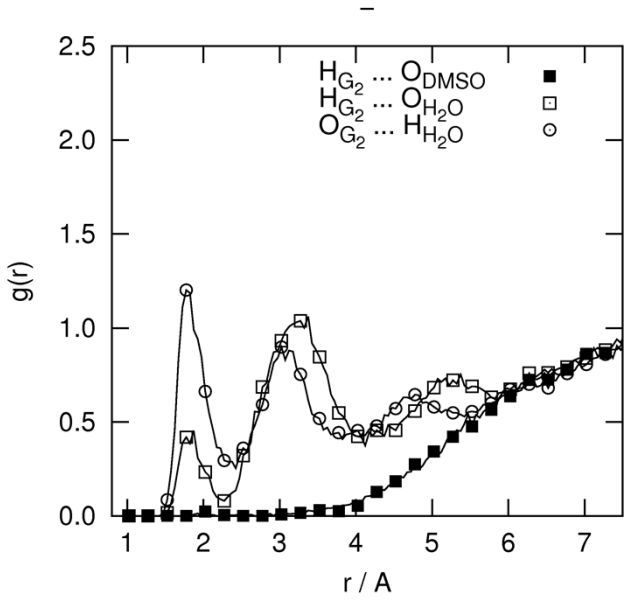
Simulation	Ionic liquid	DMSO	H_2O	Glucose
$[C_4C_1Im][OAc]$	1024	–	–	–
$[C_4C_1Im][OAc]$ + glucose	1024	–	–	16
$[C_4C_1Im][OAc]$ + DMSO	512	512	–	–
$[C_4C_1Im][OAc]$ + DMSO + glucose	512	512	–	16
$[C_4C_1Im][OAc]$ + H_2O	512	–	512	–
$[C_4C_1Im][OAc]$ + H_2O + glucose	512	–	512	16

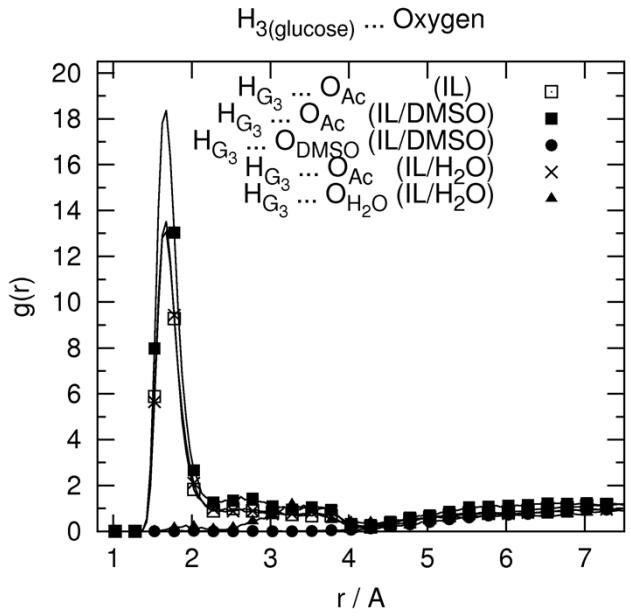
S5. Radial distribution function involving atoms of H-bonds between glucose and acetate, water and DMSO.

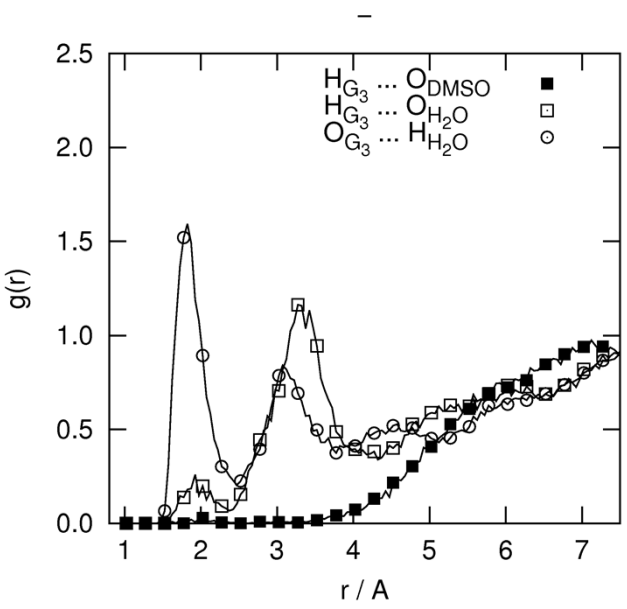


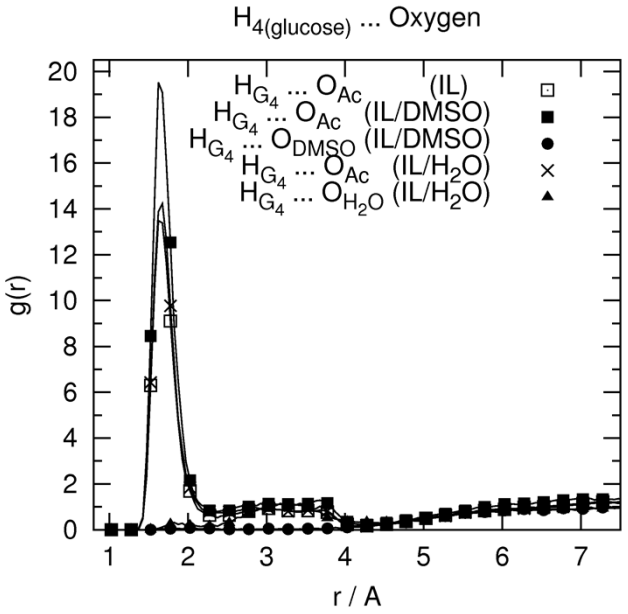


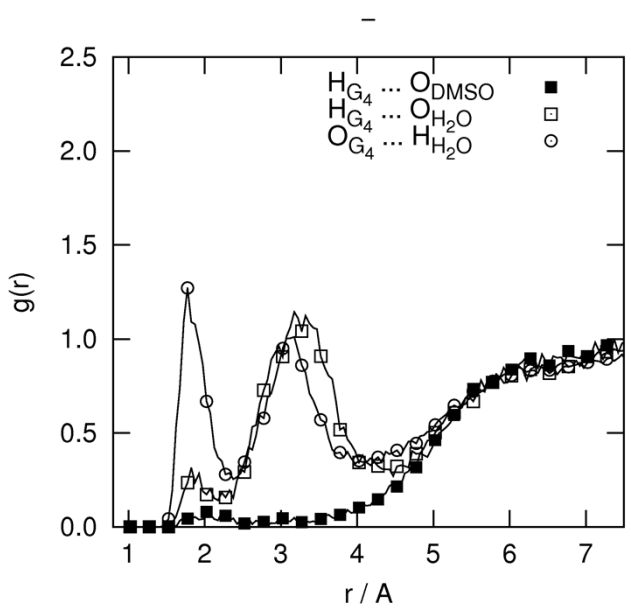


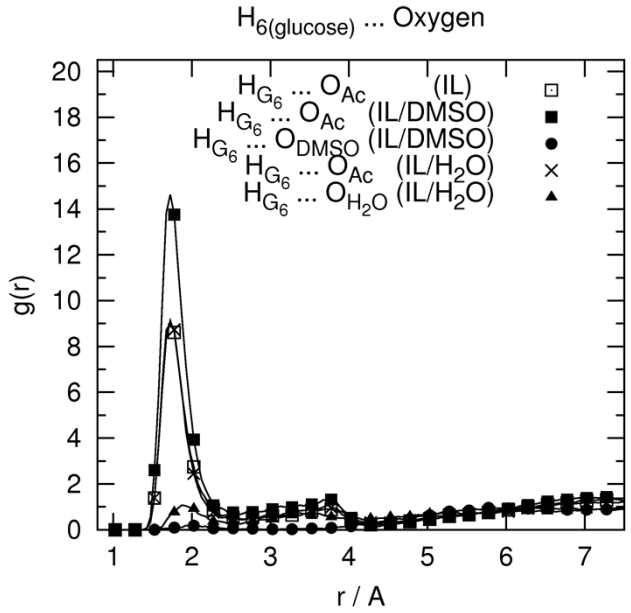


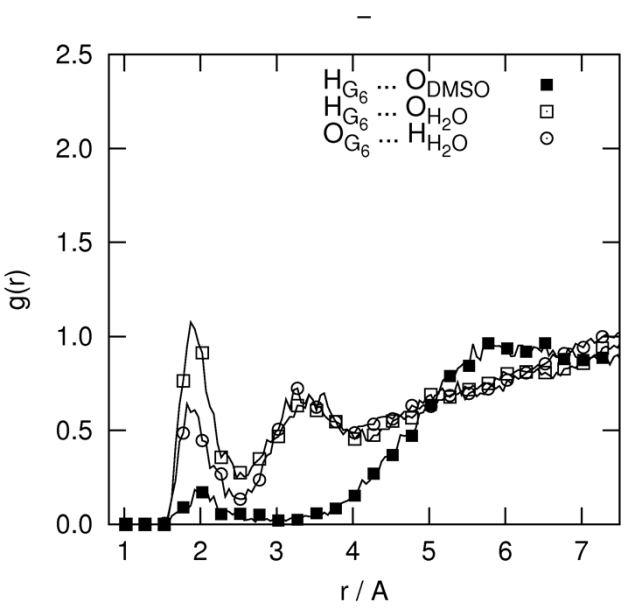

H3(glucose) ... Oxygen
HG3 ... OAc (IL)
HG3 ... OAc (IL/DMSO)
HG3 ... ODMSO (IL/DMSO)
HG3 ... OAc (IL/H2O)
HG3 ... OH2O (IL/H2O)
g(r)
r / A


–
HG3 ... ODMSO
HG3 ... OH2O
OG3 ... HH2O
g(r)
r / A


H4(glucose) ... Oxygen
HG4 ... OAc (IL)
HG4 ... OAc (IL/DMSO)
HG4 ... ODMSO (IL/DMSO)
HG4 ... OAc (IL/H2O)
HG4 ... OH2O (IL/H2O)
g(r)
r / A


–
HG4 ... ODMSO
HG4 ... OH2O
OG4 ... HH2O
g(r)
r / A


H6(glucose) ... Oxygen
HG6 ... OAc (IL)
HG6 ... OAc (IL/DMSO)
HG6 ... ODMSO (IL/DMSO)
HG6 ... OAc (IL/H2O)
HG6 ... OH2O (IL/H2O)
g(r)
r / A


–
HG6 ... ODMSO
HG6 ... OH2O
OG6 ... HH2O
g(r)
r / A