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

Supplementary Information

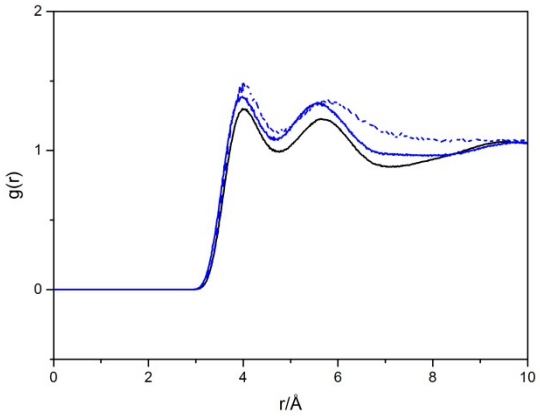

Figure S1. The methyl carbon-methyl carbon partial radial distributions for 70 mol% H_2O 2-propanol/water (dashed line) and 90 mol% H_2O 2-propanol/water (solid line) compared with neat 2-propanol methyl carbon- methyl carbon (black) at 298 K derived from the EPSR simulation.

Table S1. Lennard-Jones and Charge parameters used for the reference potential in the EPSR simulations of liquid mixtures of 2-propanol/water.

Atom type	Description	ε/ kJ mol^{-1}	σ/ Å	q/e
2-propanol				
O	O	0.711	3.12	-0.683
H_O	Alcohol-H	0	0	0.418
C_M	Methyl-C	0.276	3.5	-0.18
C_C	Tertiary-C	0.276	3.5	0.205
H_M	Methyl-H	0.126	2.5	0.06
H_C	H	0.126	2.5	0.06
Water				
O_W	O	0.65	3.16	-0.8476
H_W	H	0	0	0.4238

Table S2. Dielectric relaxation parameters obtained through fitting the model described in the manuscript to the acquired THz-TDS data.

mol% H_2O	ε_1	ε_2	ε_3	τ_3 (fs)
0	0	16.8	0.5	118
10	0.7	16.4	0.5	133
20	2.5	15.1	0.6	137
30	3.3	15.5	0.6	148
40	4.1	16.5	0.6	164
50	4.7	18.8	0.8	134
60	4.8	22.8	0.9	132
70	7.5	26.1	1.0	132
80	11.6	30.5	1.2	130
85	18.1	29.9	1.3	161
90	23.1	32.5	1.4	144
92	27.1	31.9	1.6	144
95	37.9	26.7	1.7	144
96	38.6	27.7	1.8	137
98	56.1	13.6	1.9	126
99	65.3	6.0	1.9	132
100	73.2	0	2.0	107