Supporting information

A systematic study on intradiffusion and structure of *N*, *N*-dimethylformamide-water mixtures: by experiment and molecular dynamics simulation

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Table S 1 Measured intradiffusion coefficients (in 10^{-9} m^2 s^{-1}) of water molecule in DMF-water mixtures at various temperatures, pressures, and compositions.

T (K)	x_{DMF} = 0.124					
	2 MPa	10 MPa	50 MPa	100 MPa	150 MPa	200 MPa
422.3	–	–	–	–	–	–
372.6	5.08	–	4.29	3.67	3.13	2.65
333.7	2.83	–	2.34	1.95	1.70	1.48
313.4	1.98	–	1.66	1.39	1.19	1.01
298.3	1.46	–	1.19	0.991	0.830	0.715
278.4	0.891	–	0.727	0.607	0.496	0.415
256.3	0.468	–	0.381	0.301	0.246	0.202
243.3	0.311	–	0.236	0.186	0.149	0.120
233.1	0.210	–	–	–	–	–
T (K)	x_{DMF} = 0.250					
422.3	9.22	–	–	7.22	–	–
372.6	4.73	4.61	4.19	3.79	3.48	3.20
333.7	2.22	2.18	1.98	1.79	1.62	1.50
313.4	1.34	1.31	1.19	1.07	0.966	0.886
298.3	0.839	0.826	0.747	0.668	0.604	0.549
278.4	0.425	–	0.368	0.322	0.289	0.257
256.3	0.140	–	0.121	0.104	0.0894	0.0760
243.3	0.0631	–	0.0497	0.0403	0.0336	0.0285
233.1	0.0273	–	–	–	–	–

Table S 1 (continued)

T (K)	x_{DMF} = 0.328					
	2 MPa	10 MPa	50 MPa	100 MPa	150 MPa	200 MPa
422.3	9.15	–	–	6.89	–	–
372.6	4.51	–	3.98	3.52	3.20	2.97
333.7	2.19	–	1.90	1.68	1.49	1.37
313.4	1.33	–	1.15	1.01	0.904	0.817
298.3	0.858	–	0.730	0.631	0.558	0.507
278.4	0.425	–	0.364	0.309	0.267	0.233
256.3	0.150	–	0.122	0.101	0.0820	0.0686
243.3	0.0684	–	0.0533	0.0416	0.0325	0.0260
233.1	0.0311	–	–	–	–	–
T (K)	x_{DMF} = 0.500					
422.3	8.64	–	–	6.50	–	–
372.6	4.66	4.49	3.93	3.38	2.99	2.69
333.7	2.29	2.22	1.93	1.65	1.44	1.28
313.4	1.45	1.41	1.22	1.04	0.902	0.784
298.3	0.96	0.929	0.799	0.671	0.574	0.506
278.4	0.52	0.496	0.428	0.354	0.296	0.249
256.3	0.218	0.206	0.172	0.137	0.112	0.0915
243.3	0.115	–	0.0853	0.0677	0.0526	0.0425
233.1	0.0672	–	–	–	–	–
T (K)	x_{DMF} = 0.765					
422.3	10.5	–	–	8.85	–	–
372.6	5.59	–	5.17	4.80	4.55	4.32
333.7	2.80	–	2.61	2.46	2.34	2.23
313.4	1.75	–	1.65	1.56	1.49	1.43
298.3	1.16	–	1.09	1.04	0.995	0.953
278.4	0.614	–	0.583	0.555	0.534	0.519
256.3	0.217	–	0.210	0.202	0.195	0.188
243.3	–	–	–	–	–	–
233.1	–	–	–	–	–	–

Table S 2 Measured intradiffusion coefficients (in 10^{-9} m^2 s^{-1}) of DMF molecule in DMF-water mixtures at various temperatures, pressures, and compositions.

T (K)	x_{DMF} = 0.124					
	2 MPa	10 MPa	50 MPa	100 MPa	150 MPa	200 MPa
422.3	–	–	–	–	–	–
372.6	3.55	–	2.88	2.38	2.04	1.78
333.7	2.22	–	1.76	1.46	1.24	1.07
313.4	1.64	–	1.31	1.07	0.90	0.762
298.3	1.26	–	0.999	0.816	0.678	0.571
278.4	0.848	–	0.660	0.530	0.425	0.352
256.3	0.502	–	0.381	0.293	0.230	0.181
243.3	0.339	–	0.248	0.188	0.144	0.111
233.1	0.235	–	–	–	–	–
T (K)	x_{DMF} = 0.250					
422.3	–	–	–	–	–	–
372.6	2.79	2.72	2.43	2.13	1.90	1.72
333.7	1.34	–	1.18	1.03	0.92	0.821
313.4	0.849	0.818	0.717	0.621	0.549	0.496
298.3	0.535	0.515	0.447	0.386	0.337	0.305
278.4	0.268	0.261	0.225	0.190	0.164	0.142
256.3	0.0885	–	0.0714	0.0571	0.0468	0.0380
243.3	0.0378	–	0.0288	0.0223	0.0180	0.0142
233.1	0.0165	–	–	–	–	–
T (K)	x_{DMF} = 0.328					
422.3	–	–	–	–	–	–
372.6	2.81	–	2.39	2.08	1.85	1.65
333.7	1.42	–	1.19	1.02	0.898	0.806
313.4	0.887	–	0.749	0.639	0.547	0.488
298.3	0.589	–	0.483	0.401	0.347	0.304
278.4	0.297	–	0.242	0.196	0.163	0.136
256.3	0.104	–	0.0802	0.0618	0.0492	0.0392
243.3	0.0467	–	0.0343	0.0254	0.0196	0.0152
233.1	0.0211	–	–	–	–	–
T (K)	x_{DMF} = 0.500					
422.3	–	–	–	–	–	–
372.6	3.03	2.91	2.49	2.13	1.84	1.62
333.7	1.64	1.58	1.34	1.13	0.961	0.829
313.4	1.09	1.05	0.888	0.733	0.621	0.53
298.3	0.753	0.729	0.608	0.492	0.413	0.352
278.4	0.437	0.414	0.341	0.276	0.224	0.181
256.3	0.197	–	0.148	0.113	0.0875	0.0667
243.3	0.103	–	0.0744	0.0540	0.0390	0.0287

Table S 2 (continued)

T (K)	x_{DMF} = 0.500					
	2 MPa	10 MPa	50 MPa	100 MPa	150 MPa	200 MPa
233.1	0.0609	–	–	–	–	–
T (K)	x_{DMF} = 0.765					
422.3	–	–	–	–	–	–
372.6	3.06	–	2.78	2.53	2.31	2.13
333.7	1.55	–	1.39	1.27	1.17	1.10
313.4	0.960	–	0.881	0.810	0.750	0.701
298.3	0.624	–	0.577	0.535	0.496	0.465
278.4	0.329	–	0.298	0.274	0.255	0.241
256.3	0.109	–	0.100	0.0923	0.0853	0.0802
243.3	–	–	–	–	–	–
233.1	–	–	–	–	–	–