



SUPPLEMENTARY MATERIAL TO
**Effects of solid poly (ethylene glycols) addition to the solutions
of aniline or *N,N*-dimethylaniline with water:
Experimental measurements and modelling**

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TABLE S-I. Experimental solid–liquid equilibria data at 0.1 MP for the binary systems: PEG 2050 + *N,N*-dimethylaniline, PEG 35000 + aniline and PEG 35000 + *N,N*-dimethylaniline; x_{PEG} represents mole fraction and w_{PEG} mass fraction of PEG 2050 or PEG 35000 in aniline or *N,N*-dimethylaniline; T refers to solid–liquid equilibria temperature; standard uncertainty, u , for each variable is: $u(T) = 1$ K, $u(x) = 10^{-4}$ (aniline and *N,N*-dimethylaniline), 10^{-5} (PEG 2050) or 10^{-7} (PEG 35000)

PEG 2050 + <i>N,N</i> -dimethylaniline			PEG 35000 + aniline			PEG 35000 + <i>N,N</i> -dimethylaniline		
x_{PEG}	w_{PEG}	T/K	x_{PEG}	w_{PEG}	T/K	x_{PEG}	w_{PEG}	T/K
0.0199	0.2557	298.15	0.0040	0.6015	328.15	0.0004	0.1103	312.15
0.0215	0.2710	302.15	0.0049	0.6492	329.15	0.0006	0.1578	313.15
0.0250	0.3025	304.15	0.0062	0.7010	338.15	0.0009	0.2003	315.15
0.0316	0.3557	306.15	0.0080	0.7519	341.15	0.0015	0.3043	316.15
0.0390	0.4070	307.15	0.0105	0.7995	342.15	0.0023	0.4010	321.15
0.0461	0.4498	308.15				0.0035	0.5021	326.15
0.0564	0.5028	309.15				0.0052	0.6020	330.15
0.0678	0.5516	311.15				0.0081	0.7016	335.15
0.0819	0.6014	313.15				0.0138	0.8015	339.15
0.0993	0.6509	315.15						
0.1923	0.8011	318.15						
1.0000	1.0000	330.14 ^a						

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TABLE S-II. Liquid–liquid phase demixing temperatures (cloud points) at 0.1 MPa for the system (aniline + PEG 2050 + H₂O); $x_{\text{PEG,B}}$ represents mole fraction and $w_{\text{PEG,B}}$ mass fraction of PEG 2050 in the mixed (PEG 2050 + water) binary solvent; T_{CP} is liquid-phase demixing (cloud point) temperature; $(x_{\text{H}_2\text{O}})_T$, $(x_{\text{Aniline}})_T$ and $(x_{\text{PEG}})_T$ refer to mole fractions of H₂O, aniline and PEG 2050 in ternary mixture, respectively; standard uncertainty, u , for each variable is: $u(T) = 0.3$ K, $u(x) = 10^{-4}$ (aniline and water) or 10^{-5} (PEG 2050)

$(x_{\text{Aniline}})_T$	$(x_{\text{PEG}})_T$	$(x_{\text{H}_2\text{O}})_T$	T_{CP} / K
Aniline + PEG 2050 + water ($x_{\text{PEG,B}} = 0.0058$ or 0.1138)			
0.0574	0.0055	0.9371	314.15
0.0645	0.0055	0.9300	323.15
0.0584	0.0055	0.9361	332.15
0.0551	0.0055	0.9394	342.15
0.7398	0.0015	0.2587	315.15
0.7199	0.0016	0.2785	324.15
0.6860	0.0018	0.3122	341.15
0.7049	0.0017	0.2934	335.15
0.7223	0.0016	0.2761	329.15
Aniline + PEG 2050 + water ($x_{\text{PEG,B}} = 0.0022$ or 0.0463)			
0.7334	0.0016	0.2650	321.15
0.7650	0.0005	0.2345	314.15
0.7423	0.0006	0.2571	325.15
0.7137	0.0006	0.2857	335.15
0.6841	0.0007	0.3152	344.15
0.0169	0.0022	0.9809	316.15
0.0155	0.0022	0.9823	325.15
0.0156	0.0022	0.9822	332.15
0.0222	0.0021	0.9757	341.15
Aniline + PEG 2050 + water ($x_{\text{PEG,B}} = 0.0087$ or 0.1619)			
0.7338	0.0023	0.2639	313.15
0.7000	0.0026	0.2974	324.15
0.6832	0.0028	0.3140	334.15
0.6567	0.0030	0.3403	343.15
0.1085	0.0078	0.8837	316.15
0.1098	0.0077	0.8825	323.15
0.1085	0.0078	0.8837	333.15
0.1049	0.0078	0.8873	343.15

TABLE S-III. Liquid–liquid phase demixing temperatures (cloud points) at 0.1 MPa for the system (aniline + PEG 35000 + H₂O); $x_{\text{PEG,B}}$ represents mole fraction and $w_{\text{PEG,B}}$ mass fraction of PEG 35000 in the mixed (PEG 35000 + water) binary solvent; T_{CP} is liquid-phase demixing (cloud point) temperature; $(x_{\text{H}_2\text{O}})_T$, $(x_{\text{Aniline}})_T$ and $(x_{\text{PEG}})_T$ refer to mole fractions of H₂O, aniline and PEG 35000 in ternary mixture, respectively; standard uncertainty, u , for each variable is: $u(T) = 0.4$ K; $u(x) = 10^{-4}$ (aniline and water) and 10^{-7} (PEG 35000)

$(x_{\text{Aniline}})_T$	$(x_{\text{PEG}})_T \times 10^5$	$(x_{\text{H}_2\text{O}})_T$	T_{CP} / K
Aniline + PEG 35000 + water ($x_{\text{PEG,B}} = 2.720 \times 10^{-5}$ or 0.01008)			
0.0066	2.7	0.9934	315.15
0.0072	2.7	0.9928	323.15

TABLE S-III. Continued

$(x_{\text{Aniline}})_T$	$(x_{\text{PEG}})_T \times 10^5$	$(x_{\text{H}_2\text{O}})_T$	T_{CP} / K
Aniline + PEG 35000 + water ($x_{\text{PEG,B}} = 2.720 \times 10^{-5}$ or 0.01008)			
0.0063	2.7	0.9937	332.15
0.0062	2.7	0.9938	341.15
0.7504	0.68	0.2496	324.15
0.7304	0.73	0.2696	332.15
0.6982	0.82	0.3018	345.15
0.7103	0.78	0.2897	339.15
0.7571	0.66	0.2429	313.15
0.7566	0.66	0.2434	321.15
Aniline + PEG 35000 + water ($x_{\text{PEG,B}} = 1.285 \times 10^{-4}$ or 0.04607)			
0.0139	12.7	0.9860	317.15
0.0139	12.7	0.9860	329.15
0.0152	12.7	0.9847	338.15
0.7691	2.97	0.2308	318.15
0.7594	3.09	0.2406	326.15
0.7193	3.61	0.2807	335.15
0.6804	4.11	0.3195	343.15

TABLE S-IV. Liquid–liquid phase demixing temperatures (cloud points), at 0.1 MPa, for the system (*N,N*-dimethylaniline + PEG 2050 + H₂O); $x_{\text{PEG,B}}$ represents mole fraction and $w_{\text{PEG,B}}$ mass fraction of PEG 2050 in the mixed (PEG 2050 + water) binary solvent; T_{CP} is liquid–phase demixing (cloud point) temperature; $(x_{\text{H}_2\text{O}})_T$, $(x_{\text{DMA}})_T$ and $(x_{\text{PEG}})_T$ refer to mole fractions of H₂O, *N,N*-dimethylaniline and PEG 2050 in ternary mixture, respectively; standard uncertainty, u , for each variable is: $u(T) = 0.3 \text{ K}$, $u(x) = 10^{-4}$ (*N,N*-dimethylaniline and water) or 10^{-5} (PEG 2050)

$(x_{\text{DMA}})_T$	$(x_{\text{PEG}})_T$	$(x_{\text{H}_2\text{O}})_T$	T_{CP} / K
<i>N,N</i> -Dimethylaniline + PEG 2050 + water + ($x_{\text{PEG,B}} = 0.0058$ or 0.08982)			
0.0012	0.0058	0.9930	313.15
0.0011	0.0058	0.9931	328.15
0.0023	0.0058	0.9919	341.15
0.0028	0.0058	0.9914	350.15
0.8363	0.0009	0.1628	321.15
0.8208	0.0010	0.1782	331.15
0.8006	0.0012	0.1982	340.15
0.7709	0.0013	0.2278	349.15
<i>N,N</i> -Dimethylaniline + PEG 2050 + water ($x_{\text{PEG,B}} = 0.0022$ or 0.3600)			
0.8533	0.0003	0.1464	321.15
0.8331	0.0004	0.1665	332.15
0.8130	0.0004	0.1866	340.15
0.7928	0.0005	0.2067	349.15
0.0019	0.0022	0.9959	340.15
0.0011	0.0022	0.9967	313.15
0.0012	0.0022	0.9966	329.15

TABLE S-IV. Continued

$(x_{\text{DMA}})_T$	$(x_{\text{PEG}})_T$	$(x_{\text{H}_2\text{O}})_T$	T_{CP} / K
<i>N,N</i> -Dimethylaniline PEG 2050 + water ($x_{\text{PEG,B}} = 0.0087$ or 0.1293)			
0.0068	0.0086	0.9846	343.15
0.0099	0.0086	0.9815	351.15
0.0025	0.0087	0.9888	315.15
0.0021	0.0087	0.9892	330.15
0.8128	0.0005	0.1867	333.15
0.8031	0.0029	0.1940	341.15
0.7923	0.0031	0.2046	349.15
0.8161	0.0004	0.1835	321.15

Table S-V. Liquid–liquid phase demixing temperatures (cloud points) at 0.1 MPa for the system (*N,N*-dimethylaniline + PEG 35000 + H₂O); $x_{\text{PEG,B}}$ represents mole fraction and $w_{\text{PEG,B}}$ mass fraction of PEG 35000 in the mixed (PEG 35000 + water) binary solvent; T_{CP} is liquid–phase demixing (cloud point) temperature; $(x_{\text{H}_2\text{O}})_T$, $(x_{\text{DMA}})_T$ and $(x_{\text{PEG}})_T$ refer to mole fractions of H₂O, *N,N*-dimethylaniline and PEG 35000 in ternary mixture, respectively; standard uncertainty, u , for each variable is: $u(T) = 0.4 \text{ K}$; $u(x) = 10^{-4}$ (*N,N*-dimethylaniline and water) or 10^{-7} (PEG 35000)

$(x_{\text{DMA}})_T$	$(x_{\text{PEG}})_T \times 10^5$	$(x_{\text{H}_2\text{O}})_T$	T_{CP} / K
<i>N,N</i> -dimethylaniline + PEG35000 + water ($x_{\text{PEG,B}} = 2.720 \cdot 10^{-5}$ or $w_{\text{PEG,B}} = 0.0078$)			
0.0007	2.72	0.9992	317.15
0.0007	2.71	0.9992	328.15
0.0010	2.70	0.9989	340.15
0.0014	2.70	0.9986	349.15
0.9024	0.340	0.0976	351.15
0.9579	0.10	0.0421	321.15
0.9571	0.12	0.0429	331.15
0.9444	0.15	0.0556	340.15
<i>N,N</i> -dimethylaniline PEG35000 + water ($x_{\text{PEG,B}} = 1.285 \cdot 10^{-4}$ or $w_{\text{PEG,B}} = 0.0358$)			
0.9313	0.8800	0.0686	321.15
0.9205	1.020	0.0795	331.15
0.9018	1.260	0.0982	340.15
0.8810	1.530	0.1189	351.15
0.0013	12.84	0.9986	350.15
0.0011	12.84	0.9988	321.15
0.0011	12.84	0.9988	329.15

REFERENCES

1. G. Ivanis, J. Vuksanovic, M. Calado, M. Kijevcenin, S. Serbanovic, Z. Visak, *Fluid Phase Equilib.* **316** (2012) 74.