

SUPPLEMENTARY MATERIAL TO  
**Experimental investigation and modeling of thermophysical and extraction properties of choline chloride + DL-malic acid based deep eutectic solvent**

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TABLE S-I. Experimental densities, viscosities and refractive indices for binary mixture DES (1) + methanol (2) over the temperature range between 298.15 K and 323.15 K and at atmospheric pressure; standard uncertainties,  $u$ , for each variable are:  $u(T) = 0.01$  K;  $u(p) = 5$  %;  $u(x_i) = 0.0001$ , and the combined expanded uncertainties,  $U_c$ , are  $U_c(\rho) = 4 \times 10^{-2}$  kg·m<sup>-3</sup>;  $U_c(n_D) = 9 \times 10^{-5}$  and  $U_c(\eta) = 1.0$  %, with 0.95 level of confidence ( $k \approx 2$ ); –: values out of the measuring range of the apparatus

$x_1$	$\rho / 10^3 \text{ kg} \cdot \text{m}^{-3}$	$\eta / \text{mPa s}$	$n_D$	$x_1$	$\rho / 10^3 \text{ kg} \cdot \text{m}^{-3}$	$\eta / \text{mPa s}$	$n_D$
$T=298.15 \text{ K}$							
0	0.787068	0.55577	–	0.6005	1.207312	775.01	1.46761
0.0996	0.922937	1.9947	1.37308	0.7001	1.225883	1585.5	1.47543
0.1999	1.018942	6.8703	1.40535	0.7990	1.241360	4682.3	1.48272
0.3001	1.094695	22.644	1.42847	0.8954	1.256641	11213	1.48808
0.3996	1.150458	96.521	1.44760	1	1.275061	22091	1.49378
0.4953	1.182521	246.24	1.45849	–	–	–	–
$T=303.15 \text{ K}$							
0	0.782343	0.52224	–	0.6005	1.203896	538.74	1.46632
0.0996	0.918439	1.8046	1.37152	0.7001	1.222609	1076.8	1.47414
0.1999	1.015164	5.998	1.40372	0.7990	1.238216	3027.7	1.48146
0.3001	1.090789	18.713	1.42697	0.8954	1.253599	6825.2	1.48684
0.3996	1.147090	74.434	1.44629	1	1.272033	13393	1.49256
0.4953	1.179176	181.13	1.45711	–	–	–	–
$T=308.15 \text{ K}$							
0	0.777601	0.48385	–	0.6005	1.200955	383.72	1.46504
0.0996	0.913966	1.6389	1.36978	0.7001	1.219912	752.6	1.47287
0.1999	1.011388	5.2275	1.40208	0.7990	1.235763	2012.4	1.48021
0.3001	1.087060	15.653	1.42548	0.8954	1.251382	4378.4	1.48560

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TABLE S-I. Continued

$x_1$	$\rho / 10^3 \text{ kg}\cdot\text{m}^{-3}$	$\eta / \text{mPa s}$	$n_D$	$x_1$	$\rho / 10^3 \text{ kg}\cdot\text{m}^{-3}$	$\eta / \text{mPa s}$	$n_D$
$T=308.15 \text{ K}$							
0.3996	1.143721	58.429	1.44502	1	1.269028	8995	1.49134
0.4953	1.175968	135.98	1.45573	—	—	—	—
$T=313.15 \text{ K}$							
0	0.772836	0.44514	—	0.6005	1.198299	279.56	1.46379
0.0996	0.910175	1.5016	1.36791	0.7001	1.217459	536.62	1.47160
0.1999	1.007611	4.573	1.40043	0.7990	1.233491	1372.1	1.47896
0.3001	1.083723	13.147	1.42402	0.8954	1.249263	2909.6	1.48438
0.3996	1.140361	46.505	1.44375	1	1.266047	5858.8	1.49012
0.4953	1.172761	104.1	1.45429	—	—	—	—
$T=318.15 \text{ K}$							
0	0.768039	0.41030	—	0.6005	1.194398	208.12	1.46253
0.0996	0.905188	1.3649	1.36621	0.7001	1.213636	390.96	1.47036
0.1999	1.003255	4.1027	1.39885	0.7990	1.229662	960.47	1.47772
0.3001	1.079164	11.318	1.42251	0.8954	1.245364	1973.8	1.48317
0.3996	1.137015	37.714	1.44245	1	1.263089	4120.7	1.48892
0.4953	1.169545	81.18	1.45288	—	—	—	—
$T=323.15 \text{ K}$							
0	0.763201	0.37457	—	0.6005	1.191126	158.78	1.46127
0.0996	0.899933	1.2724	1.36603	0.7001	1.210487	290.48	1.46921
0.1999	0.997821	3.6997	1.39691	0.7990	1.226518	690.72	1.47649
0.3001	1.074627	9.7934	1.42087	0.8954	1.242213	1381.4	1.48197
0.3996	1.133692	31.069	1.44120	1	1.260153	2923.8	1.48764
0.4953	1.166317	64.745	1.45159	—	—	—	—

TABLE S-II. Experimental densities, viscosities and refractive indices for binary mixture water (1) + DES (2) over the temperature range 298.15–363.15 K and at atmospheric pressure; standard uncertainties,  $u$ , for each variable are:  $u(T) = 0.01 \text{ K}$ ;  $u(p) = 5 \%$ ;  $u(x_i) = 0.0001$ , and the combined expanded uncertainties,  $U_c$ , are  $U_c(\rho) = 4 \times 10^{-2} \text{ kg}\cdot\text{m}^{-3}$ ;  $U_c(n_D) = 9 \times 10^{-5}$  and  $U_c(\eta) = 1.0 \%$ , with 0.95 level of confidence ( $k \approx 2$ ); —: out of the measuring range of the apparatus

$x_1$	$\rho \times 10^{-3} \text{ kg}\cdot\text{m}^{-3}$	$\eta \text{ mPa s}$	$n_D$	$\rho \times 10^{-3} \text{ kg}\cdot\text{m}^{-3}$	$\eta \text{ mPa s}$	$n_D$	$\rho \times 10^{-3} \text{ kg}\cdot\text{m}^{-3}$	$\eta \text{ mPa s}$	$n_D$
298.15 K			303.15 K			308.15 K			
0	1.275061	22091	—	1.272033	13393	—	1.269028	8995	—
0.1930	1.267518	8100.0	1.48865	1.264472	5343.7	1.48742	1.261449	3454.4	1.48620
0.2956	1.260061	3713.0	1.48440	1.256997	2261.8	1.48317	1.253954	1510.5	1.48195
0.3983	1.252732	1247.7	1.47943	1.249662	848.10	1.47820	1.246609	591.76	1.47697
0.4585	1.247395	695.01	1.47604	1.244312	486.27	1.47480	1.241233	349.13	1.47359
0.5142	1.240114	397.76	1.47156	1.236999	286.67	1.47034	1.233883	210.99	1.46913
0.5751	1.231732	233.95	1.46711	1.228575	185.03	1.46587	1.225548	154.05	1.46463
313.15 K			318.15 K			323.15 K			
0	1.266047	5858.8	—	1.263089	4120.7	—	1.260153	2923.8	—
0.1930	1.258448	2293.9	1.48499	1.255468	1565.4	1.48378	1.252506	1094.9	1.48258
0.2956	1.250925	1035.4	1.48073	1.247912	727.96	1.47951	1.244905	523.54	1.47830

TABLE S-II. Continued

$x_1$	$\rho \times 10^{-3}$ kg·m <sup>-3</sup>	$\eta$ mPa s	$n_D$	$\rho \times 10^{-3}$ kg·m <sup>-3</sup>	$\eta$ mPa s	$n_D$	$\rho \times 10^{-3}$ kg·m <sup>-3</sup>	$\eta$ mPa s	$n_D$
313.15 K			318.15 K			323.15 K			
0.3983	1.243561	423.15	1.47576	1.240514	309.51	1.47453	1.237467	230.93	1.47333
0.4585	1.238154	256.59	1.47236	1.235072	191.98	1.47116	1.232108	146.47	1.46995
0.5142	1.230874	159.20	1.46790	1.227897	122.92	1.46670	1.224906	96.029	1.46549
0.5751	1.222542	115.04	1.46339	1.219511	87.671	1.46214	1.21647	68.028	1.46089
328.15 K			333.15 K			338.15 K			
0	1.257025	2024.4		1.254030	1486.1		1.251035	1070.9	
0.1930	1.249562	782.49	1.48139	1.246632	571.46	1.48022	1.243709	425.43	1.47906
0.2956	1.241906	384.62	1.47709	1.23891	288.37	1.47591	1.235908	220.12	1.47472
0.3983	1.234435	175.52	1.47211	1.231526	135.65	1.47094	1.228609	106.55	1.46977
0.4585	1.229171	113.66	1.46877	1.226218	89.807	1.46756	1.223258	71.800	1.46639
0.5142	1.221912	76.184	1.46428	1.21892	61.294	1.46307	1.215921	50.154	1.46187
0.5751	1.213409	53.875	1.45966	1.210316	43.390	1.45845	1.207159	35.474	1.45725
343.15 K			348.15 K			353.15 K			
0	1.248040	813.29		1.245045	613.83		1.242050	482.51	
0.1930	1.240790	321.82	1.47793	1.237871	247.37		1.234950	193.02	
0.2956	1.232907	170.54	1.47361	1.229908	134.081		1.226909	106.84	
0.3983	1.225680	84.797	1.46892	1.222756	68.382		1.219824	55.778	
0.4585	1.220300	58.108	1.46530	1.217341	47.570		1.214383	39.214	
0.5142	1.212911	41.156	1.46071	1.209891	34.263		1.206861	28.774	
0.5751	1.203804	29.320	1.45610	1.200556	24.490		1.197423	20.652	
358.15 K			363.15 K						
0	1.239055	375.58		1.236060	300.95				
0.1930	1.232047	152.78		1.229219	123.34				
0.2956	1.223903	86.213		1.220891	70.321				
0.3983	1.216887	46.015		1.213944	38.628				
0.4585	1.211409	32.522		1.208444	27.120				
0.5142	1.203826	24.234		1.200823	19.286				
0.5751	1.194302	17.547		1.191271	14.635				

TABLE S-III. Experimental viscosities for the mixture DES + glycerol (choline chloride:dl-malic acid:glycerol in molar ratio 1:1:0.5) over the temperature range between 298.15 K and 363.15 K and at atmospheric pressure; standard uncertainties,  $u$ , for each variable are:  $u(T) = 0.01$  K;  $u(p) = 5$  %; the combined expanded uncertainty,  $U_c$ ,  $U_c(\eta) = 1.0$  %, with 0.95 level of confidence ( $k \approx 2$ )

$T / K$	$\eta / \text{mPa s}$
298.15	10271
303.15	6351.6
308.15	4032.7
313.15	2668.2
318.15	1801.7
323.15	1247.7
328.15	884.36
333.15	640.31

TABLE S-III. Continued

$T / \text{K}$	$\eta / \text{mPa s}$
338.15	472.54
343.15	355.17
348.15	271.39
353.15	210.66
358.15	165.85
363.15	133.12

TABLE S-IV. Parameters of viscosity fitting using Vogel–Fulcher–Tammann model, goodness of fit statistic  $R^2$  and energy of activation of viscous flow,  $E_{a,\eta} / \text{kJ mol}^{-1}$ , for the system DES + glycerol (choline chloride:DL-malic acid:glycerol is in mole ratio 1:1:0.5)

$T / \text{K}$	$A$	$B$	$T_0 / \text{K}$	$R^2$
	–3.5330	1612.0000	172.0000	0.9998
	$E_{a,\eta}$			
298.15	74.87	338.15	55.52	–
303.15	71.61	343.15	53.88	–
308.15	68.66	348.15	52.36	–
313.15	65.97	353.15	50.94	–
318.15	63.51	358.15	49.61	–
323.15	61.26	363.15	48.38	–
328.15	59.19	–	–	–