

Supporting Information

for

Elucidation of Molecular Interactions between DBU Based Protic Ionic Liquid and Organic Solvents: Thermophysical and Computational Studies

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Table S1 The densities, ρ and apparent molar volumes, V_ϕ of DBUTFA in DMSO and in DMF at $T =$ (293.15 to 328.15) K

m mol·kg ⁻¹	$\rho \cdot 10^{-3}$ kg·m ⁻³	$V_\phi \cdot 10^6$ m ³ ·mol ⁻¹	$\rho \cdot 10^{-3}$ kg·m ⁻³	$V_\phi \cdot 10^6$ m ³ ·mol ⁻¹	$\rho \cdot 10^{-3}$ kg·m ⁻³	$V_\phi \cdot 10^6$ m ³ ·mol ⁻¹
DBUTFA in DMSO						
	$T/K = 293.15$		$T/K = 298.15$		$T/K = 303.15$	
0.0	1.100409		1.095384		1.090370	
0.04504	1.102405	205.00	1.097409	205.22	1.092414	205.64
0.08961	1.104253	205.82	1.099288	206.03	1.094316	206.41
0.17553	1.107777	205.92	1.102832	206.31	1.097882	206.77
0.21788	1.109443	206.03	1.104504	206.47	1.099570	206.93
0.29559	1.112372	206.30	1.107459	206.75	1.102550	207.22
0.35200	1.114334	206.68	1.109439	207.14	1.104542	207.63
0.40064	1.115809	207.32	1.110915	207.82	1.106058	208.26
0.44717	1.117117	207.95	1.112255	208.42	1.107389	208.92
	$T/K = 308.15$		$T/K = 313.15$		$T/K = 318.15$	
0.0	1.085349		1.080329		1.075304	
0.04504	1.087418	205.93	1.082423	206.23	1.077425	206.48
0.08961	1.089347	206.69	1.084375	207.00	1.079382	207.47
0.17553	1.092934	207.19	1.087981	207.64	1.083032	208.04
0.21788	1.094637	207.36	1.089707	207.78	1.084777	208.18
0.29559	1.097647	207.65	1.092742	208.09	1.087838	208.51
0.35200	1.099650	208.09	1.094764	208.54	1.089876	208.98
0.40064	1.101274	208.52	1.096401	208.98	1.091537	209.41
0.44717	1.102526	209.40	1.097663	209.88	1.092802	210.35
	$T/K = 323.15$		$T/K = 328.15$			

0.0	1.070285		1.065264	
0.04504	1.072436	206.67	1.067393	207.88
0.08961	1.074429	207.60	1.069448	207.99
0.17553	1.078084	208.47	1.073133	208.90
0.21788	1.079847	208.60	1.074920	209.00
0.29559	1.082937	208.94	1.078036	209.36
0.35200	1.084989	209.43	1.080105	209.87
0.40064	1.086687	209.82	1.081813	210.28
0.44717	1.087945	210.82	1.083753	209.87

DBUTFA in DMF

	T/K = 293.15		T/K = 298.15		T/K = 303.15	
0.0	0.948907		0.944106		0.939408	
0.07650	0.954403	199.65	0.949573	200.68	0.944903	200.86
0.10275	0.956219	200.02	0.951404	200.79	0.946706	201.38
0.19838	0.962710	200.41	0.957820	201.54	0.953087	202.35
0.25465	0.966348	200.84	0.961439	201.95	0.956712	202.70
0.30145	0.969261	201.29	0.964306	202.51	0.959604	203.15
0.34303	0.971843	201.47	0.966854	202.74	0.962119	203.49
0.39857	0.975263	201.56	0.970255	202.80	0.965415	203.85
0.44631	0.978156	201.60	0.972997	203.18	0.968016	204.57
	T/K = 308.15		T/K = 313.15		T/K = 318.15	
0.0	0.934610		0.929846		0.925005	
0.07650	0.940120	201.25	0.935392	201.30	0.930554	201.86
0.10275	0.941956	201.46	0.937254	201.36	0.932395	202.17
0.19838	0.948358	202.57	0.943683	202.66	0.938983	202.44
0.25465	0.952005	202.91	0.947366	202.95	0.942629	203.09
0.30145	0.954892	203.45	0.950325	203.30	0.945505	203.85
0.34303	0.957428	203.76	0.952863	203.70	0.948020	204.35
0.39857	0.960796	203.96	0.956127	204.31	0.951417	204.56
0.44631	0.963383	204.78	0.958849	204.80	0.954247	204.80
	T/K = 323.15		T/K = 328.15			
0.0	0.920183		0.915360			
0.07650	0.925756	202.10	0.920953	202.39		
0.10275	0.927609	202.37	0.922812	202.67		
0.19838	0.934200	202.82	0.929406	203.26		
0.25465	0.937884	203.35	0.933126	203.66		
0.30145	0.940850	203.81	0.935920	204.88		
0.34303	0.943321	204.55	0.938448	205.37		
0.39857	0.946725	204.80	0.941805	205.75		
0.44631	0.949554	205.09	0.944492	206.41		

The standard uncertainties are $u(T) = 0.01$ K, $u(m) = 9.4 \cdot 10^{-6}$ mol kg⁻¹, $u(\rho) = 7.00 \cdot 10^{-3}$ kg m⁻³, $u(V_\phi) = (0.09 \text{ to } 0.01) \cdot 10^{-6}$ m³ mol⁻¹ for low and high concentration range of PIL, respectively.

Table S2 The speeds of sound, u and apparent molar isentropic compression, $K_{s,\phi}$ of DBUTFA in DMSO and in DMF at $T = (293.15 \text{ to } 328.15) \text{ K}$.

M mol·kg ⁻¹	u m·s ⁻¹	$K_{s,\phi} \cdot 10^{14}$ m ³ ·mol ⁻¹ ·Pa ⁻¹	u m·s ⁻¹	$K_{s,\phi} \cdot 10^{14}$ m ³ ·mol ⁻¹ ·Pa ⁻¹	u m·s ⁻¹	$K_{s,\phi} \cdot 10^{14}$ m ³ ·mol ⁻¹ ·Pa ⁻¹
DBUTFA in DMSO						
$T/K = 293.15$			$T/K = 298.15$		$T/K = 303.15$	
0.0	1502.04		1485.13		1468.10	
0.04504	1503.49	4.87	1486.91	4.58	1470.00	4.52
0.08961	1503.93	5.80	1487.44	5.67	1470.72	5.61
0.17553	1504.53	6.30	1488.14	6.29	1471.32	6.38
0.21788	1504.92	6.19	1488.56	6.21	1471.65	6.33
0.29559	1505.61	6.27	1489.32	6.31	1472.21	6.48
0.35200	1506.03	6.33	1489.73	6.40	1472.72	6.56
0.40064	1506.45	6.40	1490.24	6.47	1473.04	6.65
0.44717	1506.82	6.46	1490.64	6.54	1473.51	6.72
$T/K = 308.15$			$T/K = 313.15$		$T/K = 318.15$	
0.0	1451.23		1434.58		1417.83	
0.04504	1453.19	4.51	1437.80	2.94	1421.28	2.61
0.08961	1453.56	5.89	1438.09	5.24	1421.72	5.06
0.17553	1454.40	6.55	1438.77	6.36	1422.57	6.31
0.21788	1454.79	6.48	1439.06	6.39	1422.93	6.35
0.29559	1455.43	6.63	1439.73	6.59	1423.52	6.63
0.35200	1455.93	6.71	1440.12	6.73	1423.96	6.79
0.40064	1456.26	6.79	1440.52	6.82	1424.43	6.88
0.44717	1456.86	6.86	1440.81	6.95	1424.95	7.00
$T/K = 323.15$			$T/K = 328.15$			
0.0	1401.19		1384.57			
0.04504	1404.79	2.36	1389.90	-0.24		
0.08961	1405.36	4.94	1390.31	3.84		
0.17553	1406.08	6.39	1390.96	5.95		
0.21788	1406.61	6.40	1391.38	6.11		
0.29559	1407.26	6.71	1392.06	6.53		
0.35200	1407.74	6.87	1392.56	6.75		
0.40064	1408.24	6.97	1392.91	6.91		
0.44717	1408.79	7.10	1393.48	6.93		
DBUTFA in DMF						
$T/K = 293.15$			$T/K = 298.15$		$T/K = 303.15$	
0.0	1477.89		1458.51		1439.08	
0.07650	1478.05	21.03	1458.94	21.54	1439.22	22.72
0.10275	1478.27	20.82	1459.16	21.42	1439.66	22.31
0.19838	1479.35	20.30	1460.61	20.80	1440.81	21.73
0.25465	1479.96	20.09	1461.52	20.53	1441.83	21.40
0.30145	1480.63	19.87	1462.36	20.30	1442.39	21.23
0.34303	1481.10	19.75	1462.92	20.18	1443.16	21.03
0.39857	1481.90	19.58	1463.86	20.01	1443.97	20.84

0.44631	1482.49	19.46	1464.51	19.87	1444.63	20.66
	$T/K = 308.15$		$T/K = 313.15$		$T/K = 318.15$	
0.0	1419.52		1400.20		1381.39	
0.07650	1419.89	23.41	1400.23	24.79	1381.73	25.43
0.10275	1420.51	22.93	1400.52	24.48	1382.08	25.11
0.19838	1421.82	22.40	1402.17	23.48	1383.84	24.28
0.25465	1422.71	22.14	1403.36	23.08	1385.16	23.82
0.30145	1423.32	21.96	1404.43	22.78	1386.00	23.56
0.34303	1424.08	21.77	1405.41	22.53	1387.02	23.29
0.39857	1425.05	21.57	1406.33	22.31	1388.08	23.09
0.44631	1425.74	21.38	1407.28	22.10	1389.16	22.88
	$T/K = 323.15$		$T/K = 328.15$			
0.0	1362.23		1343.26			
0.07650	1362.04	27.17	1343.56	27.69		
0.10275	1362.41	26.65	1343.95	27.29		
0.19838	1363.69	25.78	1345.92	26.23		
0.25465	1364.50	25.40	1347.37	25.72		
0.30145	1365.27	25.10	1348.33	25.37		
0.34303	1365.81	24.88	1349.41	25.07		
0.39857	1366.62	24.64	1350.36	24.88		
0.44631	1367.47	24.41	1351.47	24.60		

The standard uncertainties are $u(T) = 0.01$ K, $u(m) = 9.40 \cdot 10^{-6}$ mol·kg⁻¹, $u(u) = 0.50$ m·s⁻¹,
 $u(K_{s,\phi}) = (0.73 \text{ to } 0.66) \cdot 10^{-15}$ m³·mol⁻¹·Pa⁻¹ for low and high concentration range of PIL,
respectively.

Table S3

Infinite dilution apparent molar expansibility, E_{ϕ}^{∞} , its second derivative, $(\partial^2 v_2^{\infty}/\partial t^2)_p$, and standard deviation, $\sigma(E_{\phi}^{\infty})$ of DBUTFA in DMSO and in DMF at different temperatures.

ILs		$E_{\phi}^{\infty} \cdot 10^{-6}/\text{m}^3 \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$							$\sigma(E_{\phi}^{\infty})$	$(\partial^2 V_{\phi}^{\infty}/\partial T^2)_p \cdot 10^6$ $\text{m}^3 \cdot \text{mol}^{-1} \cdot \text{K}^{-2}$
T/K	=	293.15	298.15	303.15	308.15	313.15	318.15	323.15	328.15	
DBUTFA in DMSO										
		-0.048	-0.017	0.014	0.045	0.075	0.106	0.137	0.168	0.49
DBUTFA in DMF										
		0.103	0.117	0.132	0.147	0.162	0.177	0.192	0.207	0.45