Supplementary information

The Constitutive Behavior of Ammonium Ionic Liquids: A Physiochemical Approach

*Akash Kumar Gupta and Ramesh L. Gardas**

Department of Chemistry, Indian Institute of Technology Madras, Chennai - 600 036, INDIA

*Corresponding author: Phone: +91 44 2257 4248; Fax: +91 44 2257 4202

E-mail: gardas@iitm.ac.in ; Web: http://www.iitm.ac.in/info/fac/gardas

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1) Further reading and data sources (accessed on 27 April 2015)

- Anton Paar Density Meter (DSA 5000M): http://www.anton-paar.com/corp-en/products/details/density-and-sound-velocity-meter-dsa-5000-m/density-meter/
- JASCO FTIR: http://www.jascoint.co.jp/asia/products/spectroscopy/ftir/ftir4100.html
- Bruker NMR:http://www.bruker.com/products/mr/nmr/avance-iii-hd/overview.html
- Waters ESI-MS: http://www.waters.com/waters/en_IN/Xevo-G2-XS-Tof/nav.htm?cid=134798183&locale=en_IN

2) **Table S1.** List of chemicals employed and their nature.

Component	Source	Purity	CAS Number
Benzylmethylamine	Sigma Aldrich	>97.0%	103-67-3
Benzyldimethylamine	Sigma Aldrich	>99.0%	103-83-3
Acetic acid	Merck	99.8%	64-19-7
Propionic acid	Qualizens	99.0%	79-09-4
Butanoic acid	Sigma Aldrich	>99.0%	107-92-6
Pentanic acid	Sigma Aldrich	>99.0%	109-52-4
Hexanoic acid	Sigma Aldrich	>99.0%	142-62-1
Heptanoic acid	Alfa Aesar	>98.0%	111-14-8
Octanoic acid	Alfa Aesar	>98.0%	124-07-2

3) **Table S2.** Experimental and predicted density data through group contribution approach, of BDMAACE in validation of Thermodynamic profile at different temperatures and atmospheric pressure along with AARD in correlation.

ρ/kg.m^{-3}							
T/K	**BMAPRO**	**BMABUT**	**BMAPENT**	**BMAHEX**	**BMAHEPT**	**BMAOCT**	**BDMAACE (Exp.)**
293.15	1036.587	1019.840	1002.451	989.311	978.889	968.510	1001.310
298.15	1032.281	1015.754	998.361	985.196	974.979	964.627	996.864
303.15	1027.912	1011.606	994.210	981.048	971.006	960.694	992.417
308.15	1023.500	1007.400	990.024	976.904	966.998	956.731	987.968
313.15	1019.056	1003.156	985.807	972.692	962.961	952.746	983.516
318.15	1014.576	998.878	981.560	968.440	958.898	948.737	979.057
323.15	1010.070	994.572	977.280	964.202	954.808	944.705	974.596
328.15	1005.532	990.233	972.971	959.911	950.689	940.647	970.124
333.15	1000.961	985.861	968.631	955.553	946.533	936.568	965.643
338.15	996.355	981.454	964.260	951.252	942.358	932.464	961.151
343.15	991.715	977.014	959.856	946.855	938.152	928.334	956.644
% AARD	1.219	1.118	0.048	1.014	0.183	0.127	-
T/K	**BDMAPRO**	**BDMABUT**	**BDMAPENT**	**BDMAHEX**	**BDMAHEPT**	**BDMAOCT**	**BDMAACE (Pred.)**
293.15	988.370	975.116	965.381	950.725	942.786	934.678	999.986
298.15	983.950	970.785	961.202	946.617	938.768	930.720	995.641
303.15	979.519	966.450	957.007	942.503	934.729	926.752	991.278
308.15	975.089	962.110	952.805	938.408	930.690	922.779	986.895
313.15	970.647	957.761	948.586	934.245	926.643	918.799	982.493

318.15	966.197	953.402	944.364	930.110	922.589	914.809	978.072
323.15	961.737	949.031	940.130	925.984	918.522	910.810	973.633
328.15	957.264	944.648	935.880	921.830	914.444	906.801	969.174
333.15	952.776	940.248	931.615	917.648	910.352	902.775	964.697
338.15	948.270	935.830	927.331	913.443	906.244	898.738	960.200
343.15	943.743	931.393	923.024	909.257	902.118	894.683	955.684
% AARD	0.224	0.554	0.492	0.989	0.765	0.563	0.107

***u*/m.s^{-1}**							
T/K	**BMAPRO**	**BMABUT**	**BMAPENT**	**BMAHEX**	**BMAHEPT**	**BMAOCT**	**BDMAACE**
293.15	1549.53	1534.51	1512.38	1502.60	1494.04	1485.82	1433.07
298.15	1530.76	1514.27	1492.96	1483.19	1475.61	1467.10	1413.97
303.15	1512.36	1494.44	1473.74	1464.03	1457.12	1448.62	1394.96
308.15	1494.33	1474.96	1454.78	1445.12	1438.40	1430.34	1376.11
313.15	1476.18	1455.70	1435.91	1426.36	1420.28	1412.22	1357.47
318.15	1458.56	1436.61	1417.14	1407.69	1402.30	1394.21	1339.06
323.15	1441.01	1417.61	1398.46	1389.10	1384.37	1376.29	1320.82
328.15	1423.55	1398.69	1379.81	1370.61	1366.54	1358.41	1302.67
333.15	1406.14	1379.82	1361.18	1352.17	1348.77	1340.62	1284.63
338.15	1388.69	1361.02	1342.64	1333.79	1330.94	1322.88	1266.70
343.15	1371.33	1342.27	1324.19	1315.47	1313.04	1305.21	1248.90

T/K	**BDMAPRO**	**BDMABUT**	**BDMAPENT**	**BDMAHEX**	**BDMAHEPT**	**BDMAOCT**	
293.15	1429.66	1413.13	1409.76	1406.74	1406.55	1408.60	
298.15	1410.36	1394.07	1391.48	1388.19	1388.56	1390.48	
303.15	1391.13	1375.10	1372.95	1369.81	1369.95	1372.41	
308.15	1372.11	1356.32	1354.61	1351.69	1351.83	1354.48	
313.15	1353.36	1337.78	1336.13	1333.84	1333.89	1336.75	
318.15	1334.87	1319.40	1318.15	1316.10	1316.17	1319.16	
323.15	1316.46	1301.14	1300.29	1298.45	1298.62	1301.69	
328.15	1298.17	1283.05	1282.55	1280.83	1281.18	1284.34	
333.15	1279.97	1265.07	1264.92	1263.33	1263.79	1267.11	
338.15	1261.83	1247.19	1247.38	1245.90	1246.50	1249.98	
343.15	1243.82	1229.42	1229.95	1228.60	1229.32	1232.95	

4) **Table S3.** Parameters for quadratic correlations of expeimental data

$$\rho = A_1 + B_1 T + C_1 T^2 \qquad u = A_2 + B_2 T + C_2 T^2$$

***ρ*/kg.m^{-3}**							
	BMAPRO	**BMABUT**	**BMAPENT**	**BMAHEX**	**BMAHEPT**	**BMAOCT**	**BDMAACE**
$A_1 \times 10^{-3}$	1.23	1.20	1.19	1.18	1.16	1.18	1.25
$B_1 \times 10$	-4.64	-3.96	-4.41	-4.71	-4.32	-6.72	-8.10
$C_1 \times 10^4$	-6.81	-7.24	-6.46	-5.95	-6.03	-2.06	-1.30

% AARD	6.72×10^{-4}	1.08×10^{-3}	5.36×10^{-4}	1.09×10^{-3}	6.54×10^{-4}	5.74×10^{-3}	5.89×10^{-4}
	BDMAPRO	**BDMABUT**	**BDMAPENT**	**BDMAHEX**	**BDMAHEPT**	**BDMAOCT**	
$A_1\times10^{-3}$	1.23	1.21	1.19	1.17	1.16	1.15	
$B_1\times10$	-7.49	-7.24	-6.82	-6.91	-6.76	-6.69	
$C_1\times10^4$	-2.25	-2.36	-2.58	-2.17	-2.16	-2.06	
% AARD	7.02×10^{-4}	7.03×10^{-4}	5.90×10^{-4}	1.20×10^{-3}	6.05×10^{-4}	5.04×10^{-4}	
u/m.s^{-1}							
	BMAPRO	**BMABUT**	**BMAPENT**	**BMAHEX**	**BMAHEPT**	**BMAOCT**	**BDMAACE**
$A_2\times10^{-3}$	2.89	2.95	2.80	2.81	2.77	2.75	2.82
B_2	-5.44	-5.66	-4.91	-5.11	-4.95	-4.94	-5.64
$C_2\times10^3$	2.96	2.86	1.82	2.16	2.10	2.09	3.08
% AARD	1.04×10^{-2}	1.11×10^{-2}	5.71×10^{-3}	6.17×10^{-3}	9.46×10^{-3}	5.83×10^{-3}	4.25×10^{-3}
	BDMAPRO	**BDMABUT**	**BDMAPENT**	**BDMAHEX**	**BDMAHEPT**	**BDMAOCT**	
$A_2\times10^{-3}$	2.82	2.79	2.74	2.7	2.74	2.70	
B_2	-5.65	-5.60	-5.34	-5.18	-5.39	-5.17	
$C_2\times10^3$	3.05	3.04	2.74	2.55	2.91	2.61	
% AARD	7.03×10^{-3}	3.72×10^{-3}	6.46×10^{-3}	7.38×10^{-3}	7.70×10^{-3}	2.20×10^{-3}	

5) **Table S4.** Consistency of Constitutive properties and Wada's formulism in context to ionic liquids

Benzylic Quats	***A* cal. from lit. contributions** (Wada, 1949)	**%ARD for *A* contributions**(Wada, 1949)
BMAPRO	115.7	44.59
BMABUT	124.8	43.96
BMAPENT	133.9	43.21
BMAHEX	143.0	42.55
BMAHEPT	152.1	42.09
BMAOCT	161.2	41.57
BDMAACE	116.7	44.83
BDMAPRO	125.8	44.14
BDMABUT	134.9	43.67
BDMAPENT	144.0	43.16
BDMAHEX	153.1	41.94
BDMAHEPT	162.2	41.40
BDMAOCT	171.3	40.74