Supporting Information

Systematic Study of the Thermophysical Properties of Imidazolium-Based Ionic Liquids with Cyano-Functionalized Anions

Catarina M. S. S. Neves[a], Kiki Adi Kurnia[a], João A. P. Coutinho[a], Isabel M. Marrucho[b], José N. Canongia Lopes[c], Mara G. Freire[a,b*] and Luís Paulo N. Rebelo[b]

[a]*Departamento de Química, CICECO, Universidade de Aveiro (www.ciceco.ua.pt), 3810-193 Aveiro, Portugal*

[b]*Instituto de Tecnologia Química e Biológica, UNL (www.itqb.unl.pt), Av. República, Ap. 127, 2780-901 Oeiras, Portugal*

[c]*Centro de Química Estrutural, Instituto Superior Técnico (cqe.ist.utl.pt), 1049-001 Lisboa, Portugal*

*Corresponding author

Tel: +351 234370200; Fax: +351 234370084; E-mail address: maragfreire@ua.pt.

Density

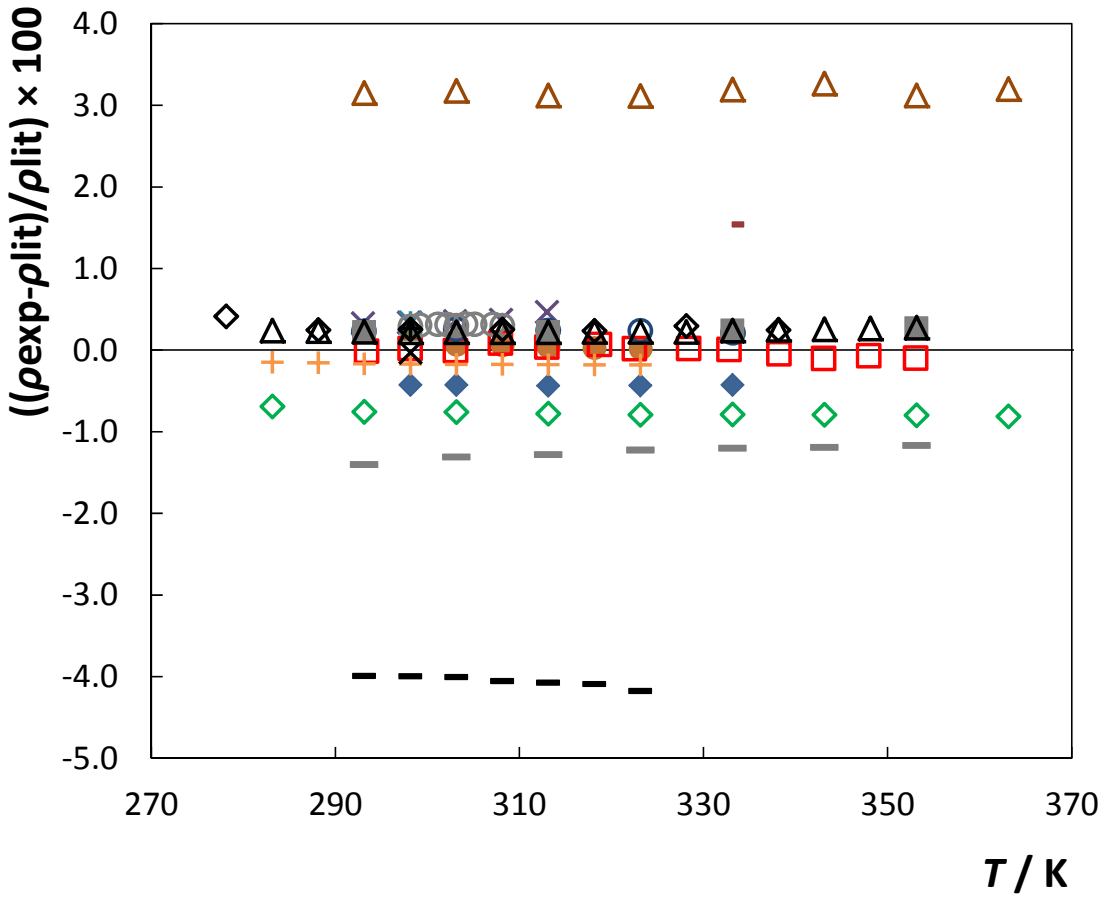

Figure S1. Relative deviations between the experimental densities measured in this work (ρexp) and those reported in literature (ρlit) as a function of temperature for the $[C_2C_1im][BF_4]$ ionic liquid: ◆, Schreiner et al.[1]; ▪, Valkenburg et al.[2]; ▲, Nishida et al.[3]; ×, Noda et al.[4]; ✳, Vila et al.[5]; ●, Wong et al.[6]; □, Klomfar et al.[7]; ◇, Shamsipur et al.[8]; —, Fredlake et al.[9], +, Sanmamed et al.[10]; ○, Currás et al.[11]; —, Gardas et al.[12]; △, Seddon et al.[13]; ○, Navia et al.[14]; ×, Stoppa et al.[15]; +, Klomfar et al.[7]; ■, Taguchi et al.[16]; ◇, Stoppa et al.[17], △, Seki et al.[18].

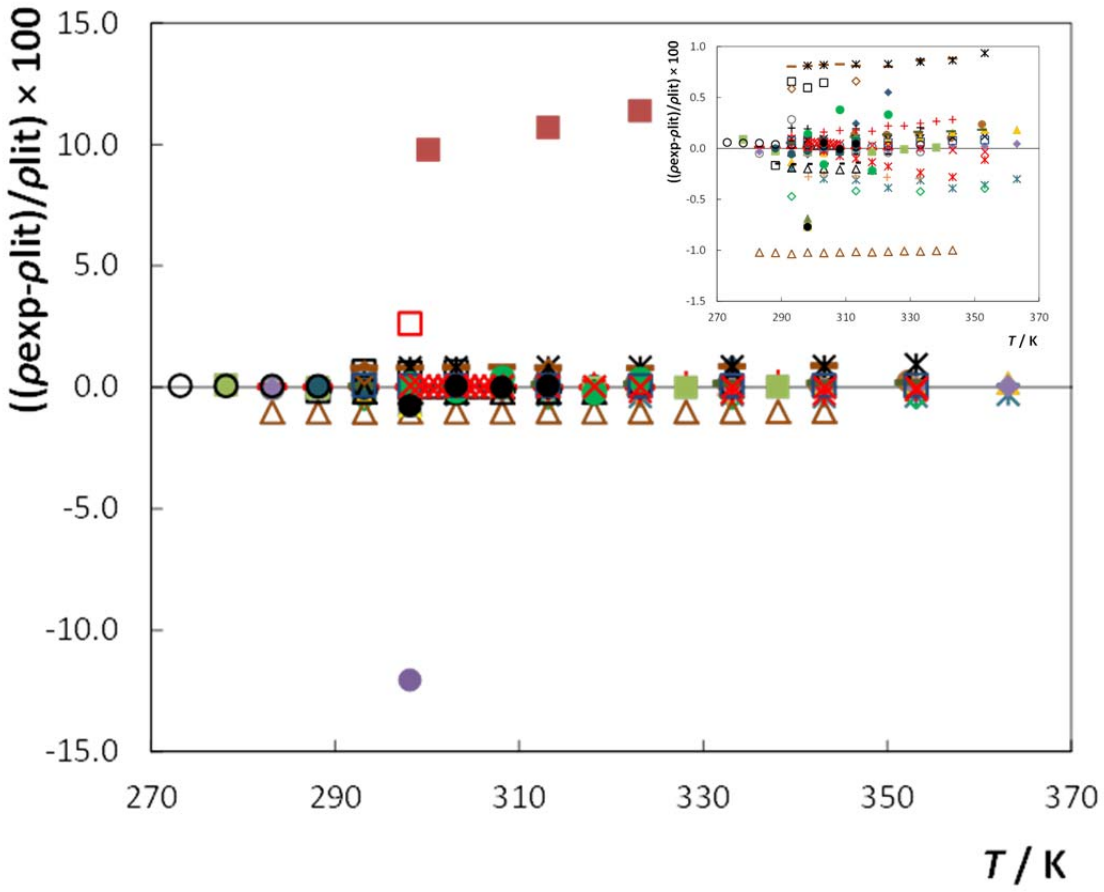

Figure S2. Relative deviations between the experimental densities measured in this work (ρexp) and those reported in literature (ρlit) as a function of temperature for the [C_4C_1im][BF_4] ionic liquid: ◆, Schreiner et al.[1]; ▪, Valkenburg et al.[2]; ▲, Nishida et al.[3]; ×, Rilo et al.[19]; ✳, Seddon et al.[13]; ●, Jacquemin et al.[20]; □, Liu et al.[21]; ◇, Tomida et al.[22]; —, Sanmamed et al.[23]; +, Gomes de Azevedo et al.[24]; ○, Iglesias-Otero et al.[25]; —, Iglesias-Otero et al.[26]; △, Kumar[27]; ○, Currás et al.[11]; ×, Taib et al.[28]; +, Tariq et al.[29]; ■, Tian et al.[30]; ◇, Malham et al.[31]; ■, Fredlake et al.[9]; ▲, Gardas et al.[32]; ●, Shekaari et al.[33]; □, Qi et al.[34]; ●, Stoppa et al.[15]; +, Jacquemin et al.[35]; —, Sanmamed et al.[10]; ▪, Tokuda et al.[36]; ◆, Sánchez et al.[37]; ■, Stoppa et al.[17]; ×, Wang et al.[38]; ✳, Zhou et al.[39]; ●, Tokuda et al.[40]; ○, Harris et al.[41]; △, Zafarani-Moattar et al.[42]; —, Huo et al.[43]; △, Navia et al.[14]; —, Jacquemin et al.[44]; △, García-Miaja et al.[45]; ✳, Huo et al.[46]; ◇, Han et al.[47]; ●, Kim et al.[48]; □, Ciocirlan et al.[49]; ×, Soriano et al.[50]; ●, Li et al.[51].

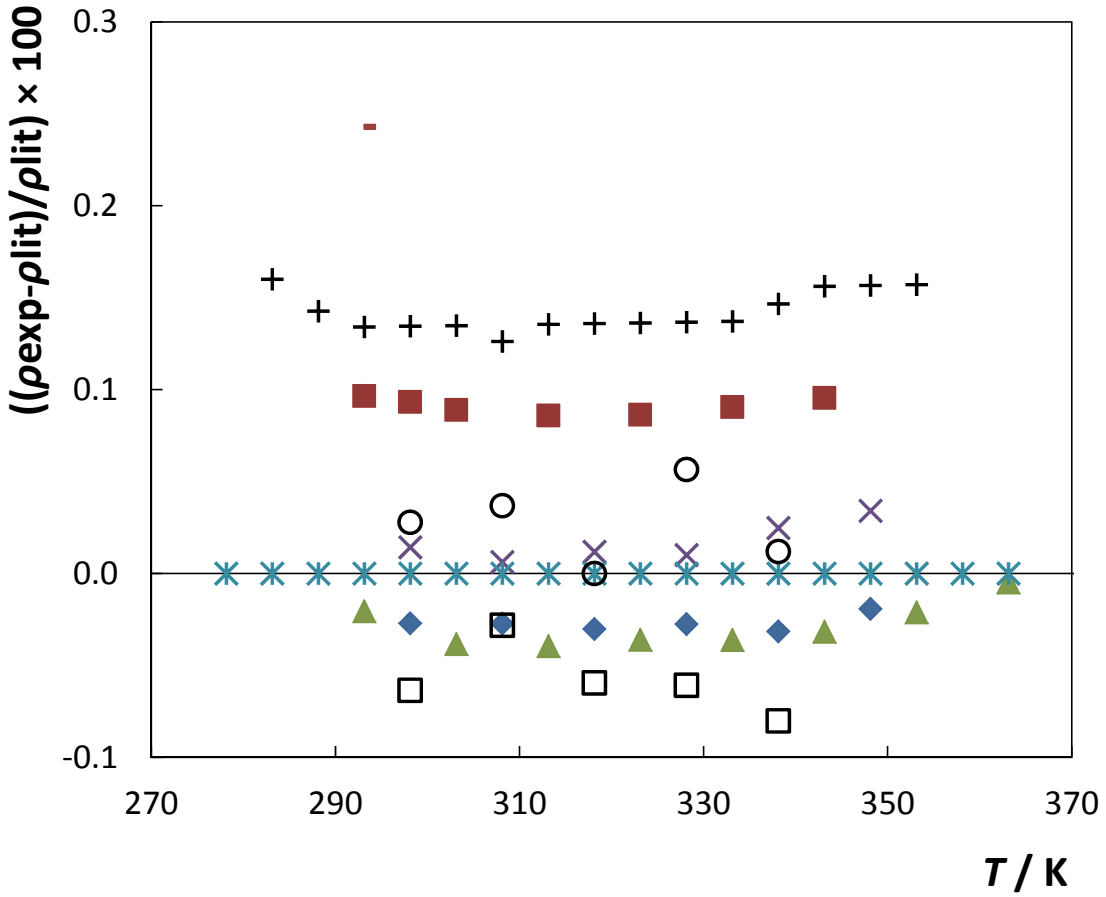

Figure S3. Relative deviations between the experimental densities measured in this work (ρexp) and those reported in literature (ρlit) as a function of temperature for the [SCN]-based ionic liquids: $[C_2C_1im]^+$, ×, Domańska et al.[52], ✳, Freire et al.[53], ■, Ficke et al.[54], ○, Królikowska et al.[55], +, Seki et al.[18]; $[C_4C_1im]^+$, ◆, Domańska et al.[56], -, Xing et al.[57], ▲, Sánchez et al.[58], □, Królikowska et al.[55].

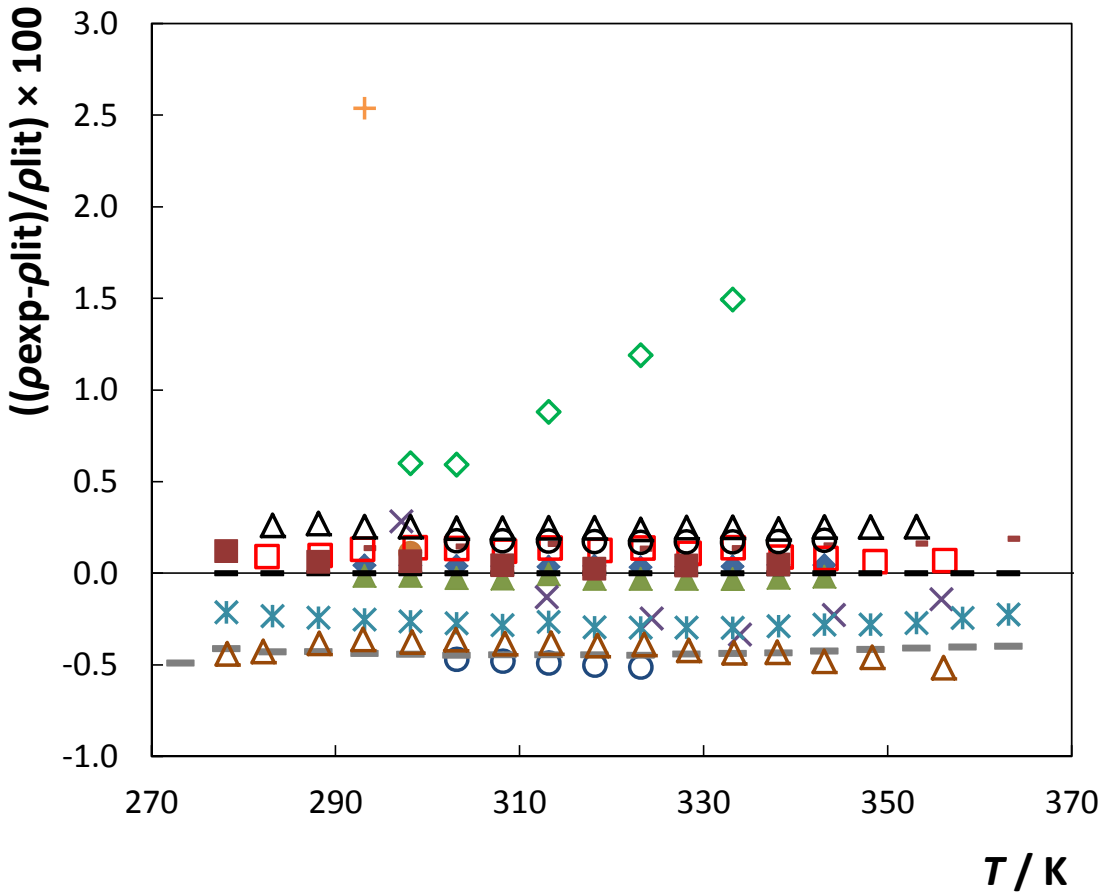

Figure S4. Relative deviations between the experimental densities measured in this work (ρexp) and those reported in literature (ρlit) as a function of temperature for the $[N(CN)_2]$-based ionic liquids: $[C_2C_1im]^+$, ◇, Schreiner et al.[1], —, Freire et al.[53], +, Yoshida et al.[59], ○, Wong et al.[6], —, Fröba et al.[60], △, Klomfar et al.[61], ○, Quijada-Maldonado et al.[62], △, Seki et al.[18]; $[C_4C_1im]^+$, -, Sánchez et al.[37], ▲, Seoane et al.[63], ×, Fredlake et al.[9], ✳, Carvalho et al.[64], ●, Stoppa et al.[15], □, Klomfar et al.[61]; $[C_6C_1im]^+$, ◆, Seoane et al.[63], ■, Zech et al.[65].

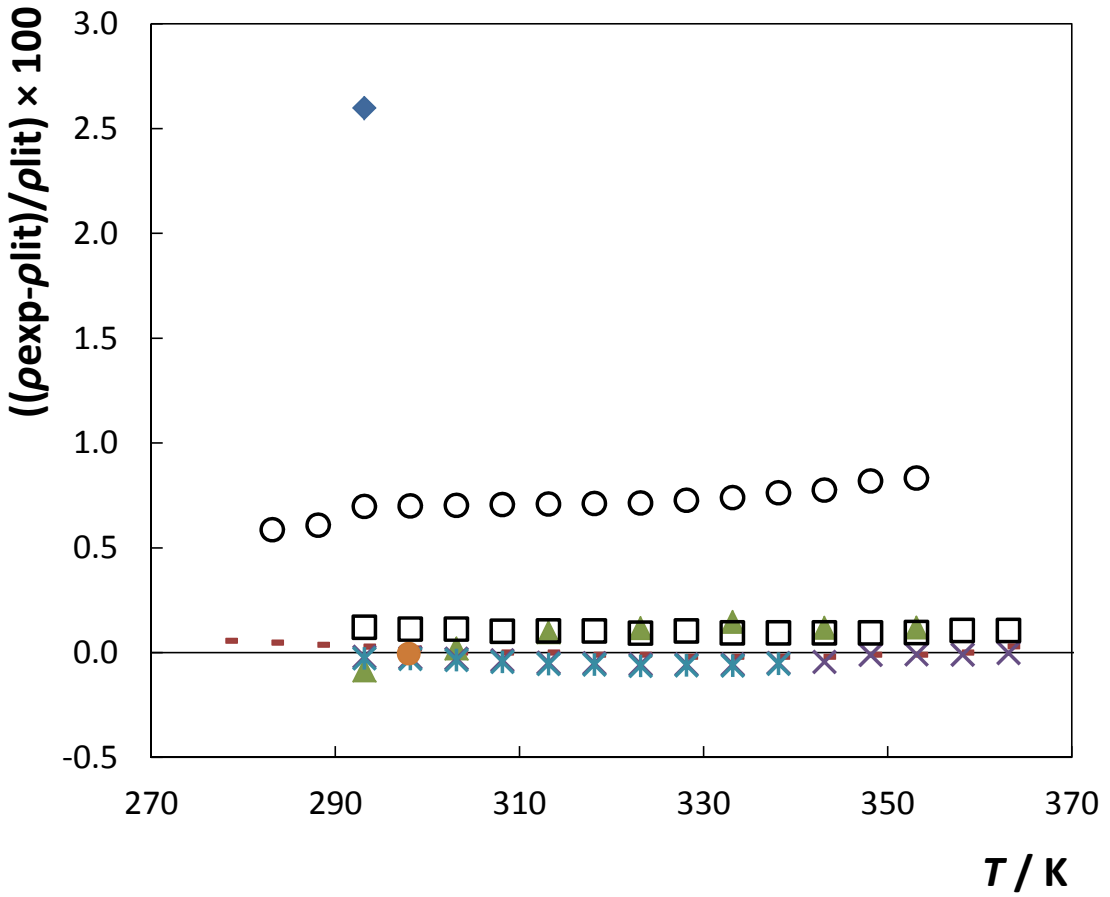

Figure S5. Relative deviations between the experimental densities measured in this work (ρexp) and those reported in literature (ρlit) as a function of temperature for the ionic liquids $[C_2C_1im][C(CN)_3]$, ◆, Yoshida et al.[59]; $[C_4C_1im][C(CN)_3]$, -, Carvalho et al.[64], ▲, Gardas et al.[12]; $[C_2C_1im][B(CN)_4]$, ×, Koller et al.[66], ✳, Tong et al.[67], ●, Mahurin et al.[68], ○, Seki et al.[18]; $[C_6C_1im][B(CN)_4]$, □, Mota-Martinez et al.[69].

Table S1. Experimental density data of the studied ILs at several temperatures and ≈ 0.1 MPa.

T / K	ρ / (kg·m^{-3})										
	$[C_2C_1im]^+$	$[C_4C_1im]^+$	$[C_2C_1im]^+$	$[C_4C_1im]^+$	$[C_6C_1im]^+$	$[C_2C_1im]^+$	$[C_4C_1im]^+$	$[C_2C_1im]^+$	$[C_6C_1im]^+$	$[C_2C_1im]^+$	$[C_4C_1im]^+$
	$[SCN]^-$		$[N(CN)_2]^-$			$[C(CN)_3]^-$		$[B(CN)_4]^-$		$[BF_4]^-$	
278.15	1129.7	1081.8	1117.9	1073.5	1041.6	1096.6	1061.4	---	1005.4	1299.1	1216.5
283.15	1126.5	1078.7	1114.3	1070.1	1038.3	1092.9	1057.9	---	1001.7	1295.1	1212.7
288.15	1123.3	1075.6	1110.9	1066.8	1035.2	1089.2	1054.4	---	998.2	1291.2	1209.0
293.15	1120.1	1072.6	1107.4	1063.5	1032.0	1085.5	1050.9	1040.1	994.6	1287.2	1205.3
298.15	1117.0	1069.5	1104.0	1060.3	1028.9	1081.9	1047.5	1036.1	990.9	1283.3	1201.7
303.15	1113.9	1066.5	1100.6	1057.0	1025.8	1078.4	1044.0	1032.1	987.3	1279.5	1198.1
308.15	1110.8	1063.6	1097.3	1053.8	1022.7	1074.8	1040.6	1028.1	983.7	1275.7	1194.5
313.15	1107.8	1060.6	1094.0	1050.9	1019.6	1071.3	1037.3	1024.1	980.1	1271.9	1191.0
318.15	1104.8	1057.7	1090.7	1047.5	1016.6	1067.8	1033.9	1020.2	976.6	1268.1	1187.4
323.15	1101.8	1054.8	1087.4	1044.4	1013.5	1064.3	1030.6	1016.3	973.0	1264.4	1183.9
328.15	1098.8	1051.9	1084.2	1041.3	1010.5	1060.8	1027.3	1012.5	969.6	1260.6	1180.5
333.15	1095.9	1049.0	1081.0	1038.2	1007.5	1057.4	1024.0	1008.7	966.1	1257.0	1177.0
338.15	1093.0	1046.1	1077.8	1035.2	1004.6	1054.0	1020.7	1005.0	962.6	1253.3	1173.6
343.15	1090.1	1043.3	1074.7	1032.2	1001.6	1050.6	1017.5	1001.3	959.2	1249.7	1170.2
348.15	1087.2	1040.5	1071.6	1029.2	999.0	1047.2	1014.3	997.9	955.8	1246.1	1166.8
353.15	1084.3	1037.7	1068.5	1026.2	996.0	1043.9	1011.1	994.2	952.4	1242.6	1163.4
358.15	1081.5	1035.0	1065.4	1023.3	993.1	1040.6	1008.0	990.5	949.1	1239.0	1160.1
363.15	1078.7	1032.2	1062.3	1020.4	990.3	1037.4	1004.9	986.9	945.8	1235.5	1156.8

Viscosity

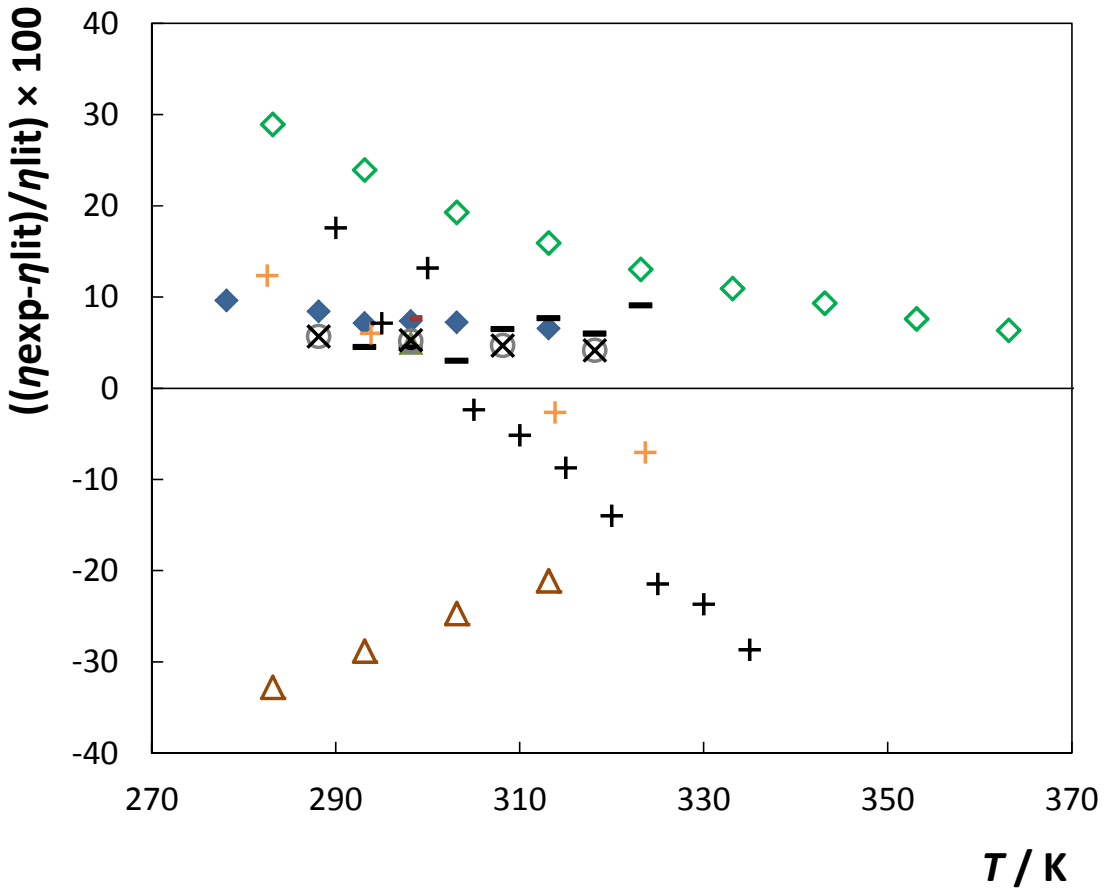

Figure S6. Relative deviations between the experimental viscosities measured in this work (ηexp) and those reported in literature (ηlit) as a function of temperature for the $[C_2C_1im][BF_4]$ ionic liquid: ◆, Schreiner et al.[1]; ▬, Valkenburg et al.[2]; ▲, Nishida et al.[3]; ◇, Shamsipur et al.[8]; —, Fredlake et al.[9], +, Sanmamed et al.[10]; △, Seddon et al.[13]; ○, Rilo et al.[70]; ×, Rilo et al.[71]; ✚, Fletcher et al.[72].

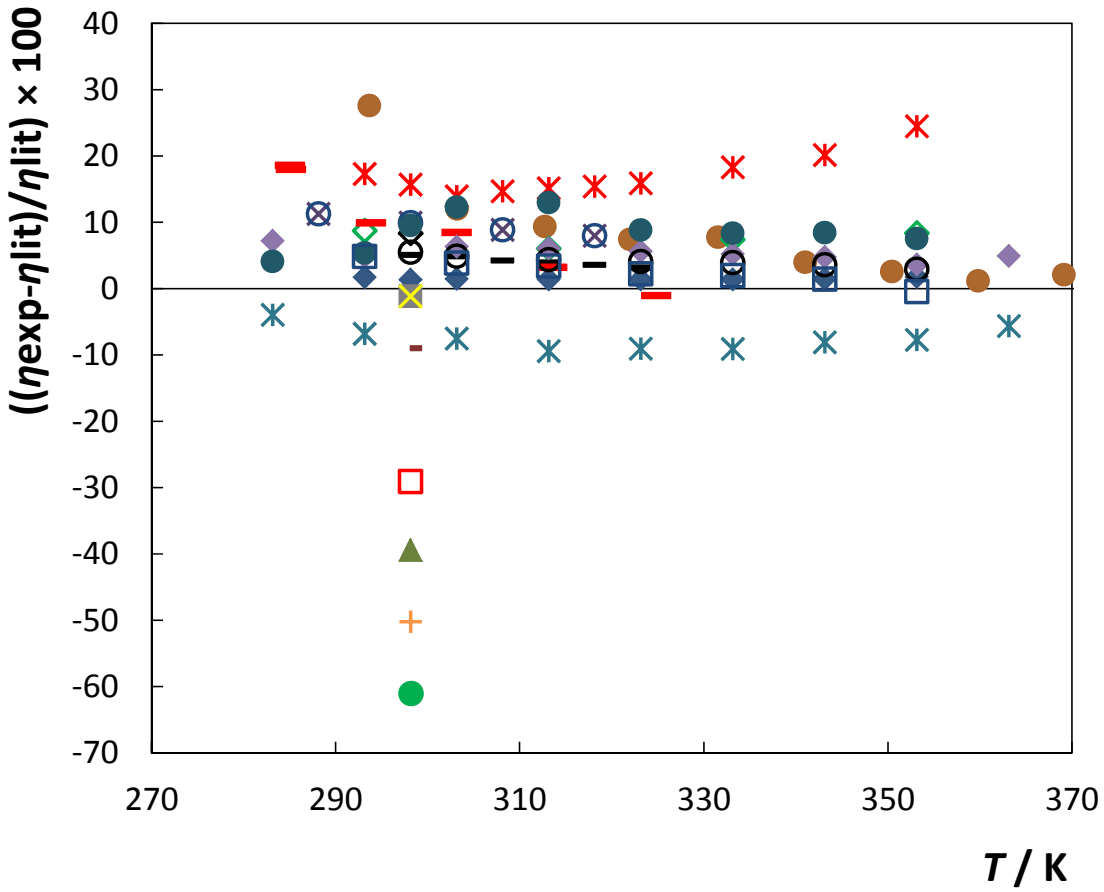

Figure S7. Relative deviations between the experimental viscosities measured in this work (ηexp) and those reported in literature (ηlit) as a function of temperature for the [C_4C_1im][BF_4] ionic liquid: ◆, Schreiner et al.[1]; -, Valkenburg et al.[2]; ▲, Nishida et al.[3]; ×, Rilo et al.[70]; ✳, Seddon et al.[13]; ●, Jacquemin et al.[20]; □, Liu et al.[21]; ◇, Tomida et al [22]; —, Sanmamed et al.[23]; +, Huddleston et al.[73]; ○, Rilo et al.[71]; ■, Tian et al.[30];◇, Malham et al.[31]; —, Sanmamed et al.[10]; ◆, Sánchez et al.[37]; ×, Wang et al.[38]; ✳, Zhou et al. [39]; ●, Tokuda et al.[40]; ○, Harris et al.[41]; ●, Kim et al.[48]; □, Ciocirlan et al.[49].

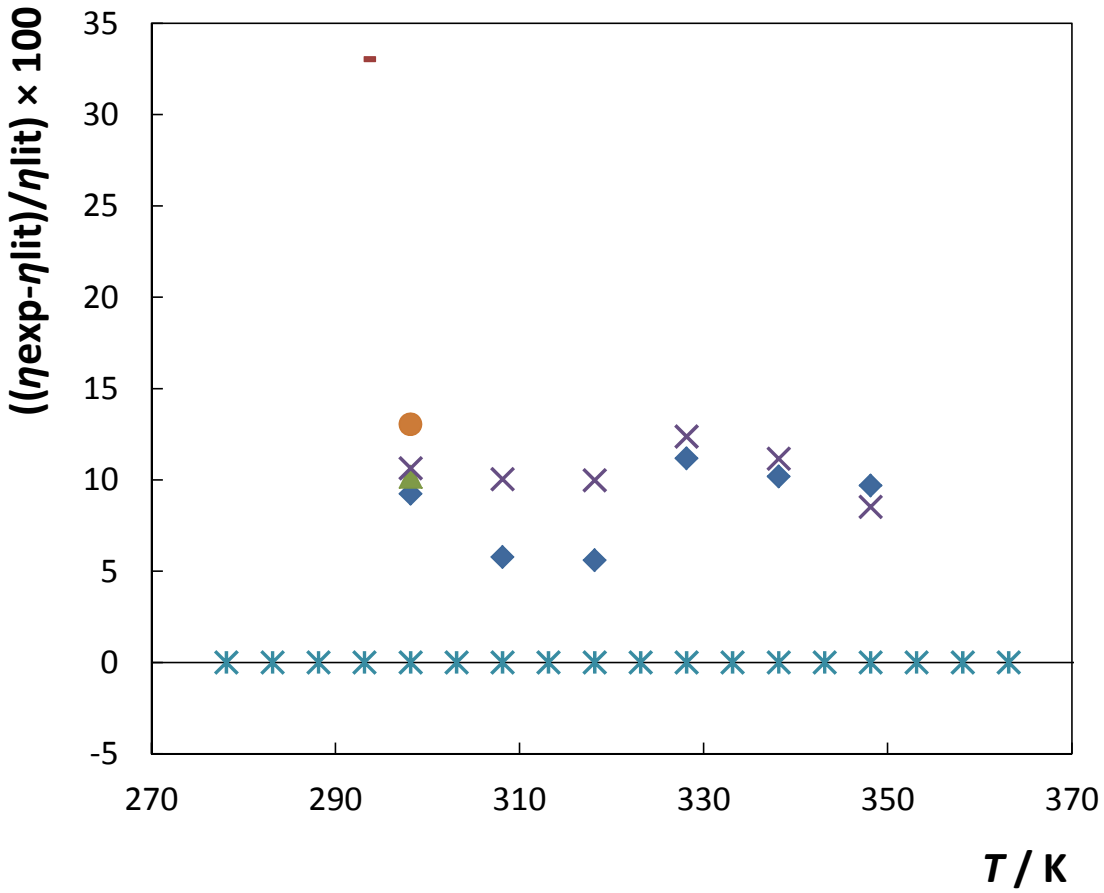

Figure S8. Relative deviations between the experimental viscosities measured in this work (ηexp) and those reported in literature (ηlit) as a function of temperature for the [SCN]-based ionic liquids: $[C_2C_1im]^+$, ×, Domańska et al.[52], ✳, Freire et al.[53]; $[C_4C_1im]^+$, ◆, Domańska et al.[56], ▬, Xing et al.[57], ▲, Rosol et al.[74], ●, Sterner et al.[75].

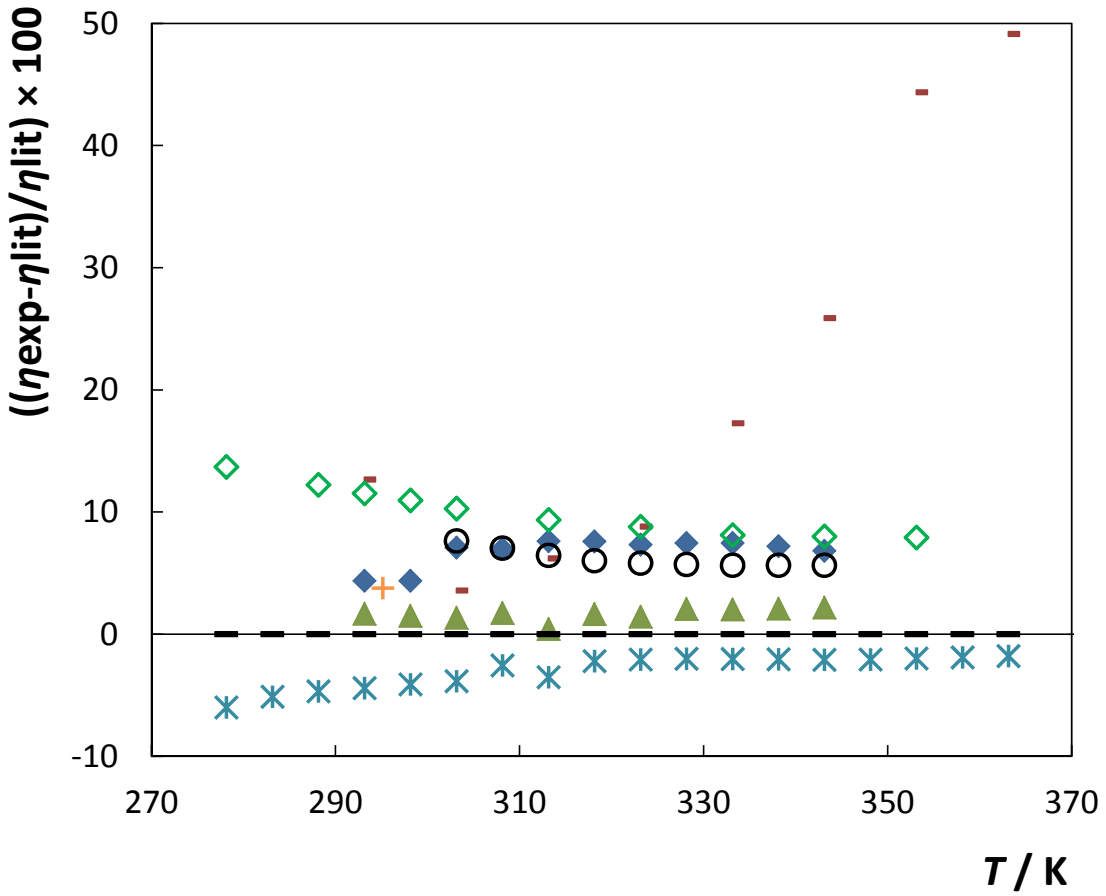

Figure S9. Relative deviations between the experimental viscosities measured in this work (ηexp) and those reported in literature (ηlit) as a function of temperature for the $[N(CN)_2]$-based ionic liquids: $[C_2C_1im]^+$, ◇, Schreiner et al.[1], —, Freire et al.[53], +, Yoshida et al.[59], ○, Quijada-Maldonado et al.[62]; $[C_4C_1im]^+$, -, Sánchez et al.[37], ▲, Seoane et al.[63], ✳, Carvalho et al.[64]; $[C_6C_1im]^+$, ◆, Seoane et al.[63].

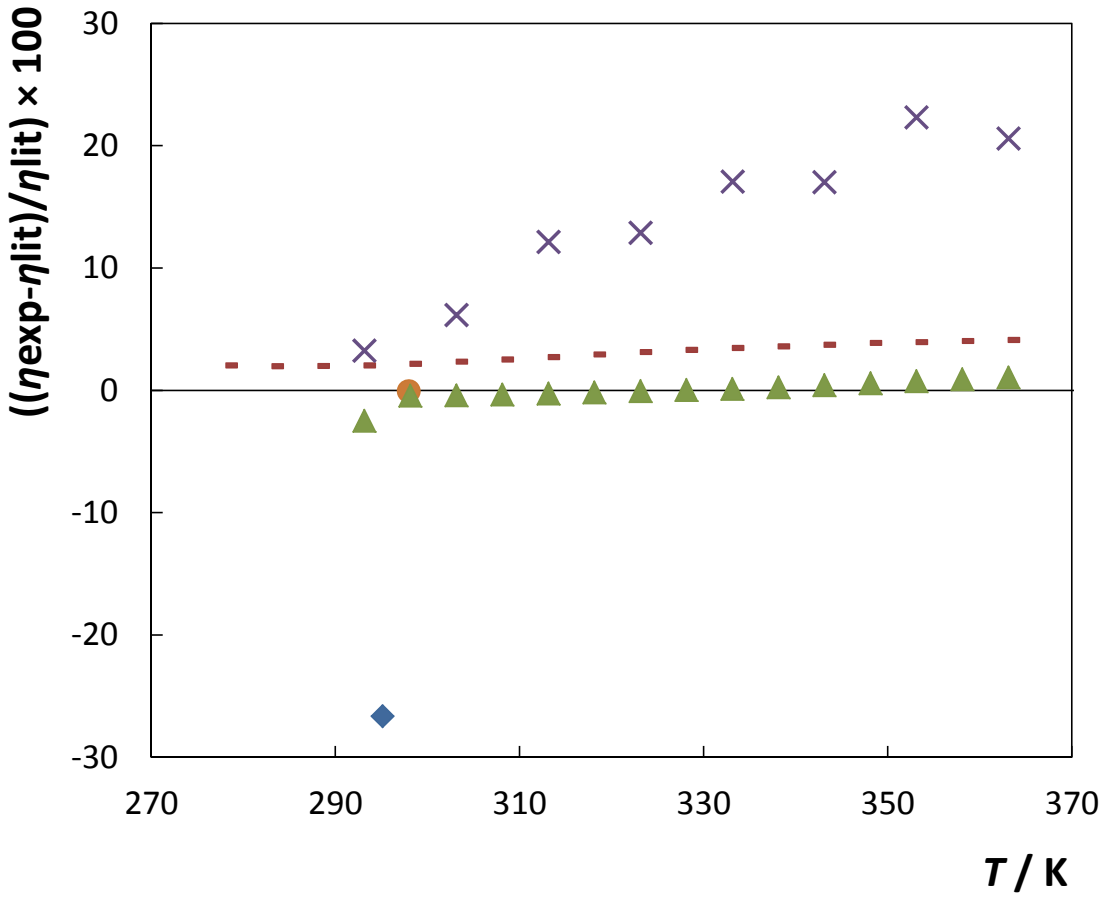

Figure S10. Relative deviations between the experimental viscosities measured in this work (ηexp) and those reported in literature (ηlit) as a function of temperature for the ionic liquids $[C_2C_1im][C(CN)_3]$, ◆, Yoshida et al.[59]; $[C_4C_1im][C(CN)_3]$, -, Carvalho et al.[64]; $[C_2C_1im][B(CN)_4]$, ×, Koller et al.[66], ●, Mahurin et al.[68]; $[C_6C_1im][B(CN)_4]$, ▲, Mota-Martinez et al.[69].

Table S2. Experimental viscosity data of the studied ILs at several temperatures and ≈ 0.1 MPa.

T / K	η / (mPa·s)										
	$[C_2C_1im]^+$	$[C_4C_1im]^+$	$[C_2C_1im]^+$	$[C_4C_1im]^+$	$[C_6C_1im]^+$	$[C_2C_1im]^+$	$[C_4C_1im]^+$	$[C_2C_1im]^+$	$[C_6C_1im]^+$	$[C_2C_1im]^+$	$[C_4C_1im]^+$
	$[SCN]^-$		$[N(CN)_2]^-$			$[C(CN)_3]^-$		$[B(CN)_4]^-$		$[BF_4]^-$	
278.15	54.573	168.34	32.507	77.152	145.54	31.536	78.193	---	173.58	95.232	376.77
283.15	43.510	123.60	26.670	59.340	107.43	25.316	58.069	---	121.03	73.940	265.99
288.15	35.360	93.178	22.233	46.642	81.423	20.729	44.419	---	87.335	58.645	193.07
293.15	29.214	71.839	18.793	37.407	63.144	17.276	34.826	22.496	64.947	47.341	143.52
298.15	24.505	56.517	16.088	30.496	49.988	14.610	27.909	18.565	49.579	38.836	109.05
303.15	20.793	45.283	13.916	25.272	41.320	12.517	22.784	15.552	38.757	32.306	84.532
308.15	17.858	36.883	12.159	21.231	33.782	10.850	18.915	13.205	30.927	27.217	66.722
313.15	15.493	30.490	10.718	17.843	28.087	9.5022	15.934	11.315	25.136	23.191	53.542
318.15	13.560	25.545	9.5187	15.533	23.646	8.3963	13.598	9.8094	20.763	19.966	43.615
323.15	11.970	21.658	8.5175	13.491	20.089	7.4787	11.738	8.5903	17.399	17.349	36.015
328.15	10.642	18.565	7.6735	11.819	17.309	6.7102	10.236	7.5939	14.767	15.208	30.110
333.15	9.5283	16.065	6.9511	10.437	15.031	6.0584	9.0062	6.7539	12.678	13.424	25.456
338.15	8.5821	14.026	6.3268	9.2800	13.153	5.5031	7.9880	6.0567	10.996	11.940	21.744
343.15	7.7727	12.344	5.7883	8.3073	11.579	5.0261	7.1378	5.4650	9.6246	10.682	18.752
348.15	7.0758	10.947	5.3188	7.4837	10.104	4.6132	6.4201	4.9607	8.4939	9.6114	16.317
353.15	6.4717	9.7696	4.9095	6.7850	9.0265	4.2536	5.8093	4.5258	7.5527	8.6952	14.303
358.15	5.9453	8.7757	4.5485	6.1846	8.0983	3.9385	5.2853	4.1441	6.7608	7.9083	12.630
363.15	5.4846	7.9265	4.2292	5.6666	7.3109	3.6610	4.8330	3.8104	6.0895	7.2248	11.227

Refractive Indices

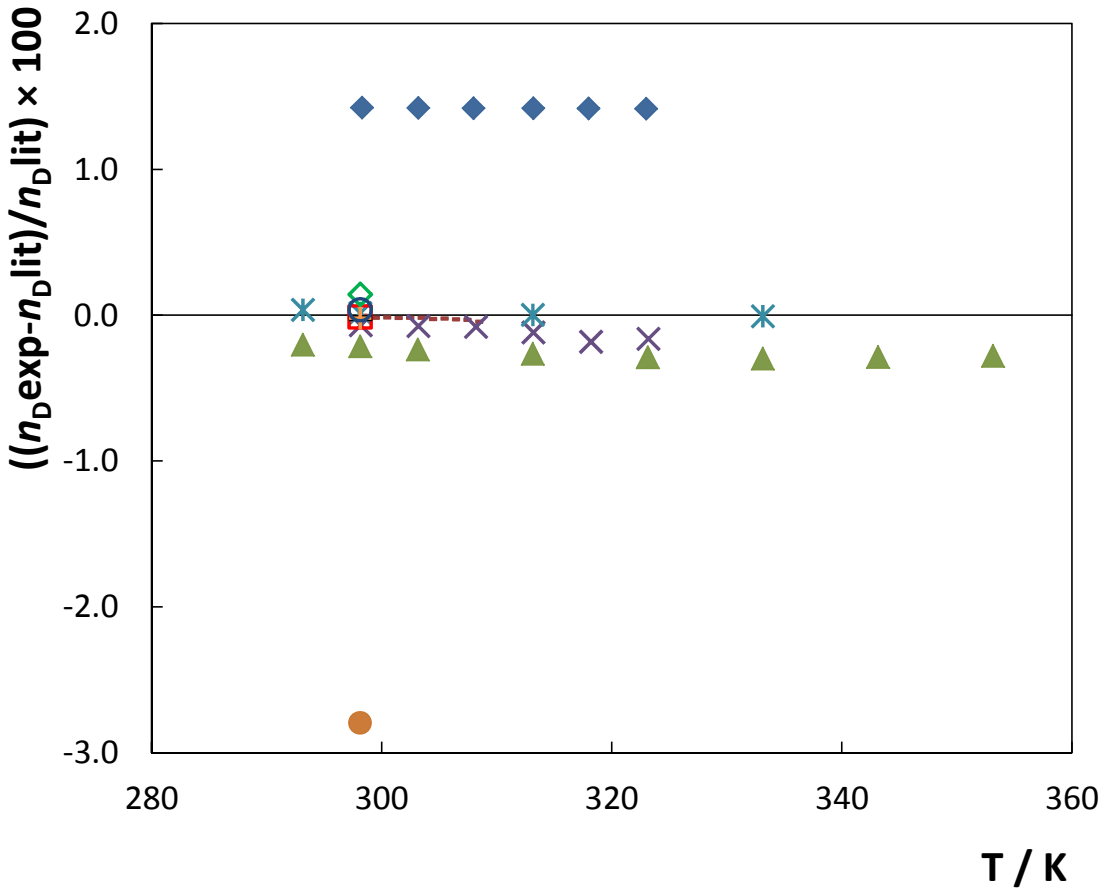

Figure S11. Relative deviations between the experimental refractive indices measured in this work ($n_D$exp) and those reported in literature ($n_D$lit) as a function of temperature for the [C_4C_1im][BF_4]: ◆, Kim et al.[76]; ▪, Soriano et al.[50]; ▲, Taib et al.[28]; ×, Kim et al.[48]; ✳, Tariq et al.[29]; ●, Liu et al.[21]; □, Iglesias-Otero et al.[25]; ◇, Kumar[27]; —, Hernández-Fernández et al.[77]; +, Malham et al.[31]; ○, Rilo et al.[78].

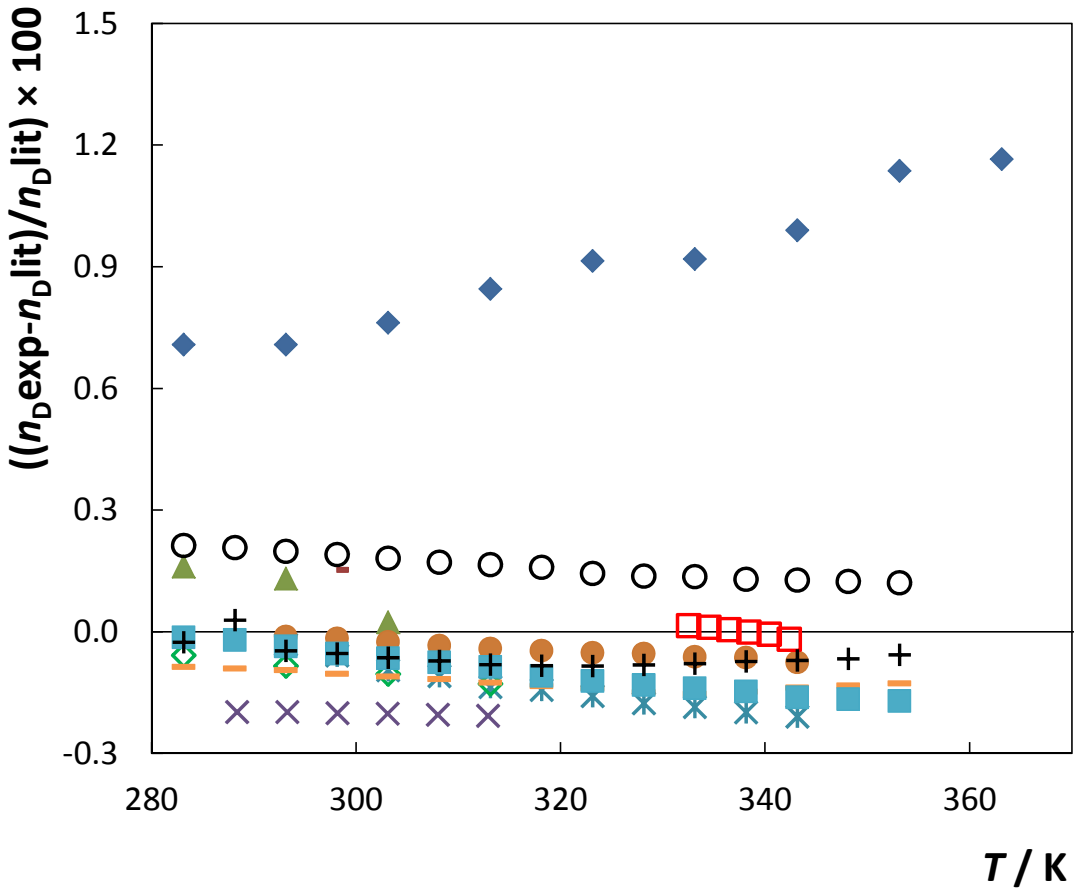

Figure S12. Relative deviations between the experimental refractive indices measured in this work ($n_D$exp) and those reported in literature ($n_D$lit) as a function of temperature for the ionic liquids: $[C_2C_1im][BF_4]$, ◆, Shamsipur et al.[8], -, Rilo et al.[78], ○, Seki et al.[18]; $[C_2C_1im][N(CN)_2]$, ▲, Fröba et al.[60], ×, Freire et al.[53], —, Seki eta al.[18]; $[C_4C_1im][N(CN)_2]$, ✳, Seoane et al.[63]; $[C_6C_1im][N(CN)_2]$, ●, Seoane et al.[13]; $[C_2C_1im][SCN]$, □, Freire et al.[53], ■, Seki et al.[18]; $[C_2C_1im][B(CN)_4]$, ◇, Koller et al.[66].

Table S3. Experimental refractive index data of the ILs studied at several temperatures and ≈ 0.1 MPa.

T / K	n_D										
	$[C_2C_1im]^+$	$[C_4C_1im]^+$	$[C_2C_1im]^+$	$[C_4C_1im]^+$	$[C_6C_1im]^+$	$[C_2C_1im]^+$	$[C_4C_1im]^+$	$[C_2C_1im]^+$	$[C_6C_1im]^+$	$[C_2C_1im]^+$	$[C_4C_1im]^+$
	$[SCN]^-$		$[N(CN)_2]^-$			$[C(CN)_3]^-$		$[B(CN)_4]^-$		$[BF_4]^-$	
283.15	1.55578	1.54370	1.51642	1.51371	1.50866	1.51821	1.51343	---	1.45779	1.41846	1.42560
288.15	1.55417	1.54234	1.51468	1.51202	1.50713	1.51626	1.50977	---	1.45609	1.41716	1.42434
293.15	1.55242	1.54090	1.51298	1.50996	1.50554	1.51427	1.50838	1.44868	1.45435	1.41580	1.42302
298.15	1.55064	1.53945	1.51121	1.50800	1.50393	1.51236	1.50649	1.44686	1.45260	1.41445	1.42171
303.15	1.54898	1.53799	1.50955	1.50588	1.50222	1.51042	1.50463	1.44499	1.45086	1.41310	1.42033
308.15	1.54732	1.53651	1.50787	1.50404	1.50050	1.50852	1.50277	1.44316	1.44912	1.41175	1.41885
313.15	1.54567	1.53499	1.50619	1.50205	1.49880	1.50665	1.50096	1.44134	1.44741	1.41042	1.41751
318.15	1.54387	1.53348	1.50453	1.50016	1.49701	1.50482	1.49918	1.43960	1.44569	1.40913	1.41622
323.15	1.54221	1.53179	1.50293	1.49835	1.49521	1.50300	1.49747	1.43791	1.44402	1.40771	1.41490
328.15	1.54059	1.53030	1.50127	1.49650	1.49350	1.50121	1.49579	1.43627	1.44233	1.40644	1.41364
333.15	1.53903	1.52808	1.49962	1.49478	1.49180	1.49949	1.49417	1.43465	1.44071	1.40517	1.41235
338.15	1.53746	1.52707	1.49809	1.49305	1.49017	1.49784	1.49255	1.43307	1.43904	1.40391	1.41108
343.15	1.53582	1.52559	1.49658	1.49136	1.48848	1.49617	1.49103	1.43146	1.43745	1.40271	1.40982
348.15	1.53431	1.52408	1.49509	1.48975	1.48694	1.49455	1.48955	1.42989	1.43592	1.40148	1.40862
353.15	1.53282	1.52252	1.49367	1.48816	1.48541	1.49293	1.48809	1.42840	1.43437	1.40027	1.40741

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