Supplementary Material (ESI) for New Journal of Chemistry

Electrochemical methodology for determination of imidazolium ionic liquids (solids at room temperature) properties: Influence of the temperature

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Supplementary Information

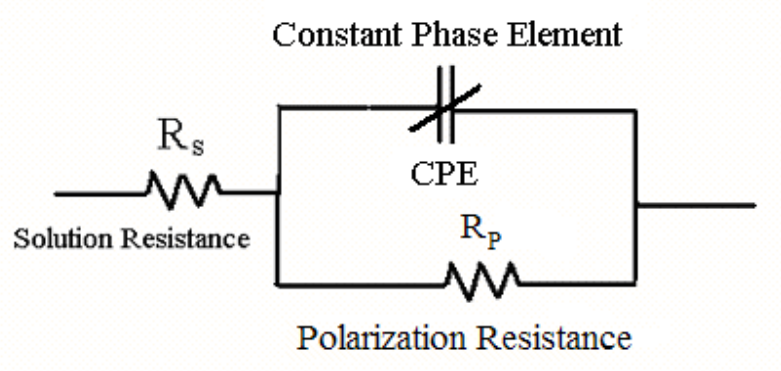

Figure S1. Proposed equivalent circuit for the platinum/IL interface.

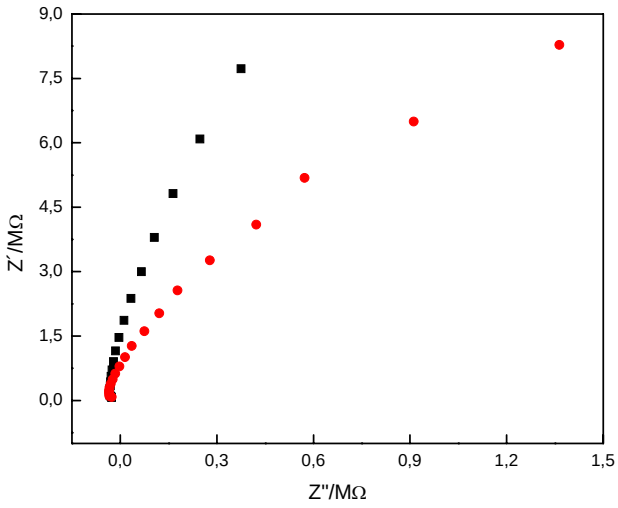

Figure S2. Nyquist diagram of **3** $[C_2O_2MIm][Cl]$ at 32 °C under a pure argon atmosphere (black points) and pure oxygen atmosphere (red points).

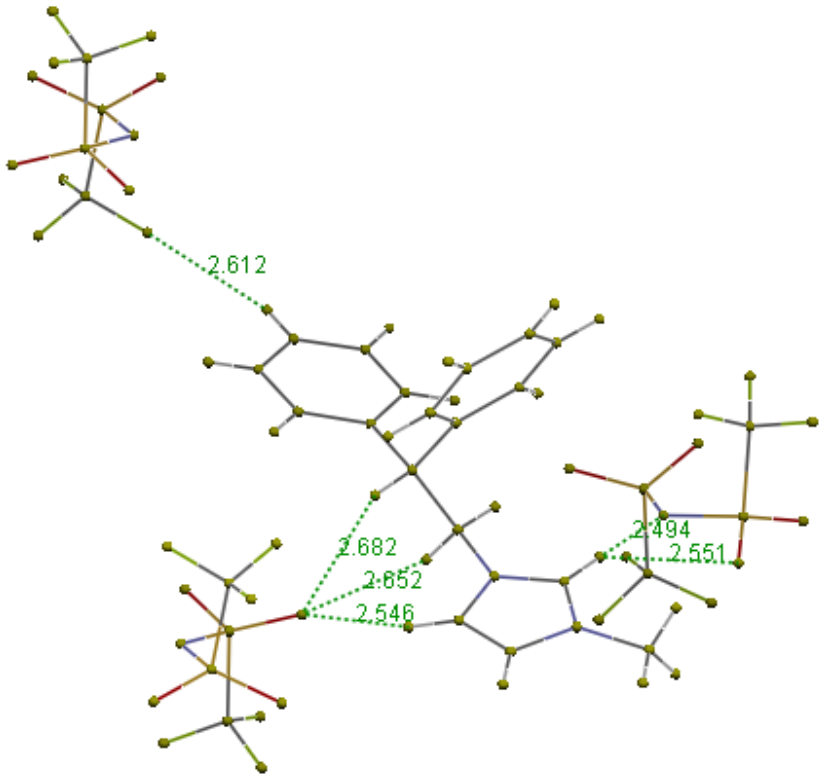

Figure S3. Mercury view of **2a** [Ph_2C_2MIm][NTf_2] showing supramolecular interactions at room temperature.

Table S1. Supramolecular interactions in the solid state of **2a** [Ph_2C_2MIm][NTf_2] at room temperature.

D	H	A	d D-H (Å)[a]	d H-A (Å)[a]	d D-A (Å)[a]	Angles DHA (°)
C15	H15	F6A[b]	0.930	2.612	3.389	141.42
C2	H2	N3[c]	0.930	2.494	2.494	155.23
C2	H2	O12[c]	0.930	2.551	2.551	138.38
C4	H4	O11[d]	0.929	2.546	3.255	133.37
C1	H1A	O11[d]	0.971	2.652	3.258	120.84
C5	H5	O11[d]	0.980	2.682	3.325	123.42

[a] d = distance. [b] Symmetry transformation used to generate equivalent atoms: 1.5-x, 1/2+y, 1.5-z. [c] Symmetry transformation used to generate equivalent atoms: 1-x, -y, 1-z. [d] Symmetry transformation used to generate equivalent atoms: 0.5+x, 0.5-y, -0.5+z.

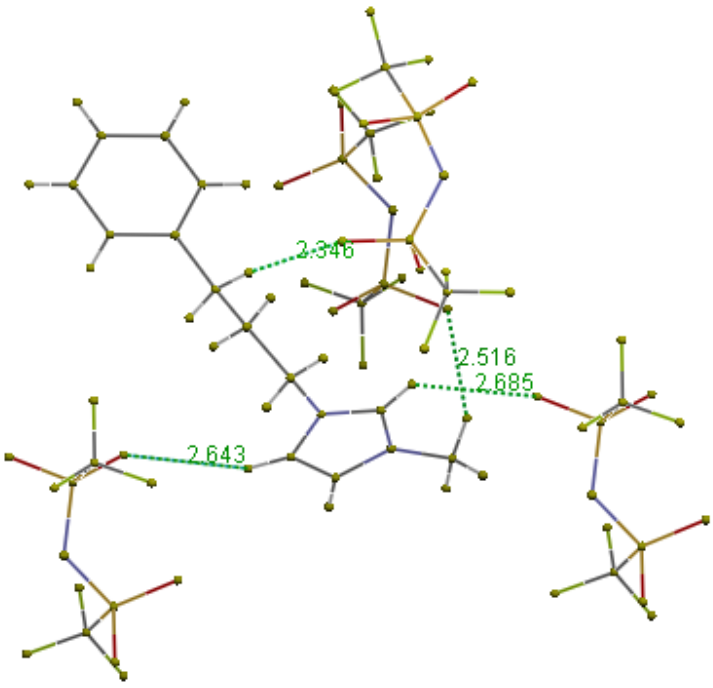

Figure S4. Mercury view of **2b** [PhC_3MIm][NTf_2] showing supramolecular interactions at room temperature.

Table S2. Supramolecular interactions in the solid state of **2b** [PhC_3MIm][NTf_2] at room temperature.

D	H	A	d D-H (Å)[a]	d H-A (Å)[a]	d D-A (Å)[a]	Angles DHA (°)
C6	H6C	O18[b]	0.960	2.516	3.392	151.74
C2	H2	O18[c]	0.930	2.685	3.492	133.24
C9	H9A	O25[d]	0.970	2.346	3.302	168.94
C4	H4	O19[b]	0.930	2.643	3.520	157.45

[a] d = distance. [b] Symmetry transformation used to generate equivalent atoms: -x, 0.5+y, 0.5-z. [c] Symmetry transformation used to generate equivalent atoms: -x, 0.5+y, 0.5-z. [d] Symmetry transformation used to generate equivalent atoms: x,y,z.

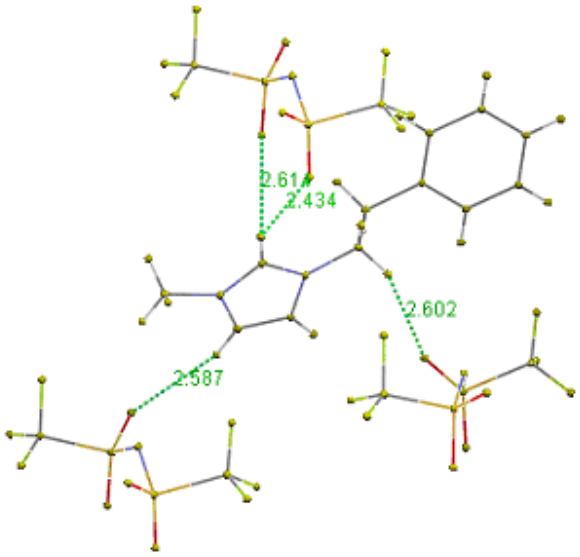

Figure S5. Mercury view of **2c** [PhC_2Mim][NTf_2] showing supramolecular interactions at room temperature.

Table S3. Supramolecular interactions in the solid state of **2c** [PhC_2Mim][NTf_2] at room temperature.

D	H	A	d D-H (Å)[a]	d H-A (Å)[a]	d D-A (Å)[a]	Angles DHA (°)
C2	H2A	O22[b]	0.970	2.602	3.408	140.75
C5	H5	O12[c]	0.930	2.587	3.475	159.70
C3	H3	O11[d]	0.930	2.614	3.781	135.61
C3	H3	O21[d]	0.930	2.434	3.623	141.05

[a] d = distance. [b] Symmetry transformation used to generate equivalent atoms: 0.5 -x, 0.5+y, 0.5-z. [c] Symmetry transformation used to generate equivalent atoms: -x, 2-y, -z. [d] Symmetry transformation used to generate equivalent atoms: 1-x, 2-y, -z.

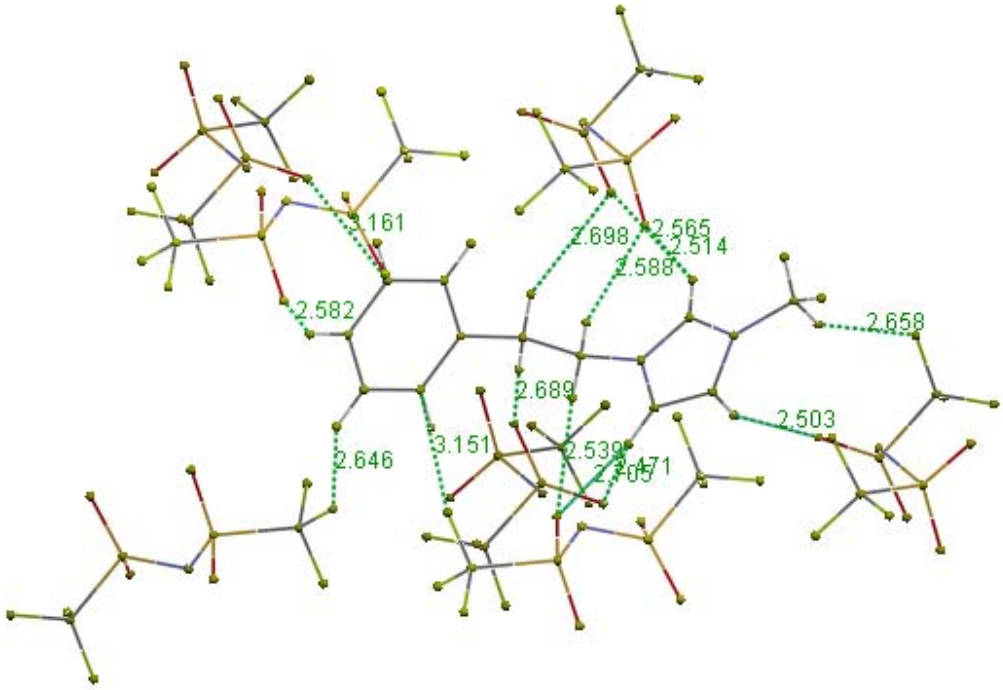

Figure S6. Mercury view of **2c** [PhC_2Mim][NTf_2] showing supramolecular interactions at -100 °C.

Table S4. Supramolecular interactions in the solid state of **2c** [PhC_2Mim][NTf_2] at -100 °C.

D	H	A	d D-H (Å)[a]	d H-A (Å)[a]	d D-A (Å)[a]	Angles DHA (°)
C9	H9	O4[b]	0.950	2.471	3.209	134.53
C10	H10	O4[c]	0.950	2.503	3.400	157.41
C12	H12A	F4[c]	0.981	2.658	3.553	151.89
C7	H7B	O3[b]	0.991	2.689	3.643	161.93
C9	H9	O1[d]	0.950	2.705	3.359	126.66
C3	H3	O2[e]	0.950	2.582	3.316	134.32
C4	H4	F2[f]	0.950	2.646	3.236	120.67
C7	H7A	O3[g]	0.990	2.698	3.495	137.73
C8	H8A	O2[g]	0.989	2.588	3.499	153.16
C11	H11	O2[g]	0.950	2.514	3.333	144.50
C11	H11	O3[g]	0.950	2.565	3.042	111.29
C8	H8B	O1[d]	0.990	2.539	3.344	138.39
C2	O4	S2[h]	3.161	1.427	4.442	148.55
C5	F1	C13[d]	3.151	1.329	4.055	124.52

[a] d = distance. [b] Symmetry transformation used to generate equivalent atoms: 1-x, 1-y, 1-z. [c] Symmetry transformation used to generate equivalent atoms: 1+x, y, z. [d] Symmetry transformation used to generate equivalent atoms: 0.5+x, 0.5-y, -0.5+z. [e] Symmetry transformation used to generate equivalent atoms: -0.5+x, 0.5-y, -0.5+z. [f] Symmetry transformation used to generate equivalent atoms: 0.5-x, 0.5+y, 0.5-z. [g] Symmetry transformation used to generate equivalent atoms: x, y, z. [h] Symmetry transformation used to generate equivalent atoms: -x, 1-y, 1-z.

Table S5. Crystallographic data for imidazolium ILs **2a-c**.

	2a (25 °C) $[Ph_2C_2Mim][NTf_2]$	**2b** (25 °C) $[PhC_3Mim][NTf_2]$	**2c** (25°C) $[PhC_2Mim][NTf_2]$	**2c** (-100 °C) $[PhC_2Mim][NTf_2]$
formula	$C_{20}H_{19}F_6N_3O_4S_2$	$C_{15}H_{17}F_6N_3O_4S_2$	$C_{14}H_{15}F_6N_3O_4S_2$	$C_{14}H_{15}F_6N_3O_4S_2$
M	543.5	481.44	467.41	467.41
crystal system	monoclinic	monoclinic	monoclinic	monoclinic
space group	*P*21/n	*P*21/c	P21/n	P21/n
a [E_1]	10.0301(9) Å	11.1807(2)	9.9583(4)	9.7783(9)
b [E_1]	18.862(2) Å	14.8585(3)	15.4739(6)	15.2038(16)
c [E_1]	12.979(1)	12.8594(3)	13.1044(5)	12.8926(14)
β [ºC]	93.289(6)	105.50	92.897(6)	92.951(6)
Z	4	4	4	4
V [$Å^3$]	2451.3(4)	2058.66(7)	2016.73(17)	1914.2(3)
ρcalcd [g/cm^3]	1.47	1.553	1.539	1.622
T [K]	173	173	173	173
θ range [ºC]	3-30	2-29	2-25	2-30
μ [mm]	0.294	0.339	0.056	0.362
reflections measured	29841	36755	17169	23008
final R1, ωR2[I>2 σ (I)]	0.078, 0.2326	0.092, 0.295	0.1012, 0.3344	0.0432, 0.1127