Supplementary information

Silica ionogels for proton transport

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Single-crystal X-ray structure analyses for [PmimSO$_3$H][PTS] : Details of the crystal data, data collection and refinement are given in Table S1. The diffraction intensities were collected with graphite-monochromatized Mo Kα radiation. Data collection and cell refinement were carried out using a Bruker Kappa X8 APEX II diffractometer. The temperature of the crystal was maintained at the selected value (200K) by means of a 700 series Cryostream cooling device to within an accuracy of ±2 K. Intensity data were corrected for Lorenz-polarization and absorption factors. The structures were solved by direct methods using SHELXS-97[1] and refined against F^2 by full-matrix least-squares methods using SHELXL-97[2] with anisotropic displacement parameters for all non-hydrogen atoms. All calculations were performed by using the Crystal Structure crystallographic software package WINGX.[3] The structure was drawn using ORTEP3.[4] All hydrogen atoms were located on a difference Fourier map and introduced into the calculations as a riding model with isotropic thermal parameters.

Table S1. Crystal data and structure refinement for the ionic liquid [PmimSO$_3$H][PTS]

Empirical formula	**C_{28} H_{40} N_4 O_{12} S_4**
Crystal size (mm^3)	0.20 x 0.14 x 0.02
Formula weight (g mol^{-1})	752.92
Temperature (K)	200 (2)
Wavelength (Å)	0.71073
Crystal system	monoclinic
Space group	*P* 2_1/n
Unit cell dimensions	
a (Å)	8.8902(3)
b (Å)	38.4841(12)
c (Å)	10.2135(3)
α (°)	90
β (°)	103.6130(10)
γ (°)	90
V (Å^3)	3396.19(19)
Z	4
$D_{calc.}$ (Mg.m^{-3})	1.467
Absorption coefficient (mm^{-1})	0.347
F (0 0 0)	1584
Index ranges	-12 < h < 12, -55 < k < 55, -13 < l <
Reflection collected	58 561
Independent reflections (Rint)	9 232 (0.0390)
Observed reflections [*I > 2σ(I)*]	6 451
Refinement method	Full matrix least squares on F^2
Final *R* indices [*I > 2σI*]	*R1* = 0.0433, *wR2* = 0.0971
Final *R* indices [*all data*]	*R1* = 0.0729, *wR2* = 0.1100
S	1.011
$(\Delta/\sigma)_{max}$	0.004
$(\Delta\ \rho)_{max,\ min}$ [e Å^{-3}]	0.321 ; -0.368

Table S2. Selected bond distances (Å) and angles (°) in the ionic liquid [PmimSO_3H][PTS].*

	Distance/angle		**Distance/angle**
S1-O1(H)	1.5001(14)	S4-O10	1.4285(16)
S1-O2	1.4450(14)	S4-O11	1.4301(15)
S1-O3	1.4310(14)	S4-O12(H)	1.5168(15)
S2-O4	1.4326(13)	S3-O7(H)	1.4925(14)
S2-O5(H)	1.5020(13)	S3-O8	1.4292(16)
S2-O6	1.4435(13)	S3-O9	1.4321(15)
O3-S1-O2	116.97(9)	O10-S4-O11	117.33(10)
O3-S1-O1	112.11(8)	O10-S4-O12	107.35(9)
O2-S1-O1	106.91(8)	O11-S4-O12	110.57(10)
O3-S1-C1	107.78(8)	O10-S4-C22	109.33(10)
O2-S1-C1	106.39(8)	O11-S4-C22	107.52(9)
O1-S1-C1	106.01(8)	O12-S4-C22	103.95(9)
O4-S2-O6	116.71(9)	O8-S3-O9	115.54(10)
O4-S2-O5	112.01(8)	O8-S3-O7	110.36(10)
O6-S2-O5	106.87(8)	O9-S3-O7	110.67(9)
O4-S2-C8	108.04(8)	O8-S3-C15	107.37(10)
O6-S2-C8	106.42(8)	O9-S3-C15	108.67(9)
O5-S2-C8	106.17(8)	O7-S3-C15	103.46(8)

* All esds *are* estimated using the full covariance matrix.

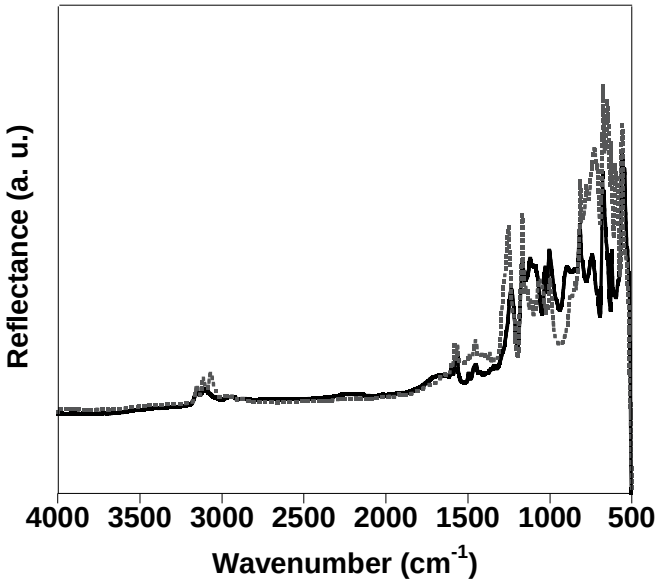

Figure S1. Infrared spectra of the as-synthesized IL (black straight line) and of the crystallized IL (grey dotted line).

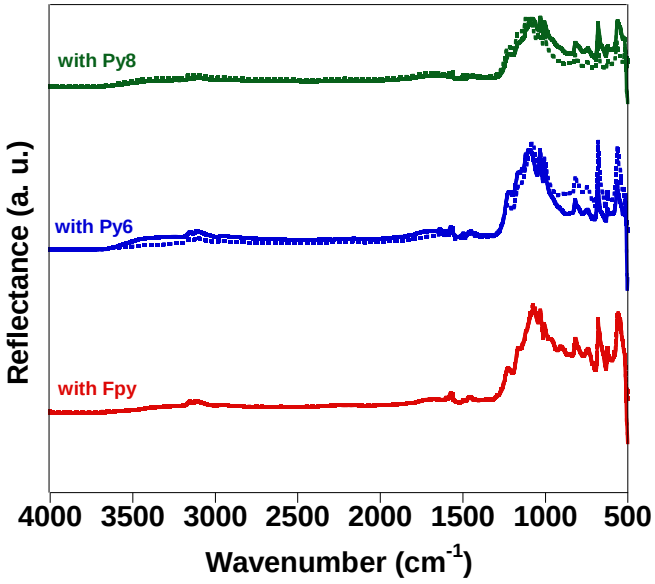

Figure S2. Infrared spectra before (dotted line) and after treatment at 120° C for 2 hours under N_2 stream (straight line) of the ionogels Fpy/IL (red), Py6/IL (blue), and Py8/IL (green).

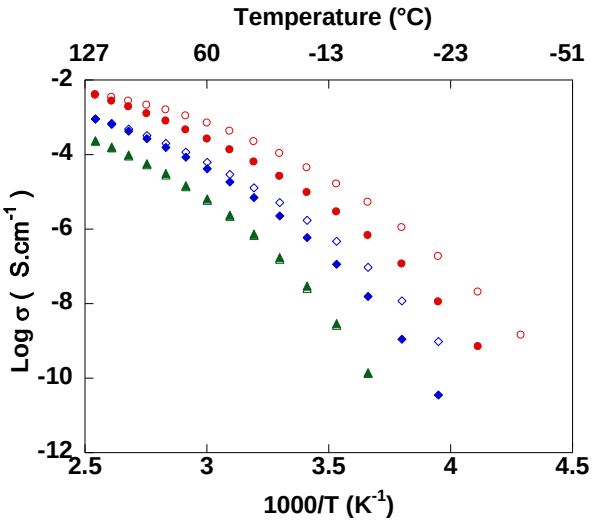

Figure S3. Conductivity vs. temperature during heating (open symbols) and cooling (closed symbols) of Fpy/IL as-synthesized (red circles), after drying under vacuum one night at 55°C (blue lozenges) and after drying 2 hours at 120° C under N_2 stream (green triangles).

References

1. G. M. Sheldrick, SHELXS-97, Program for Crystal Structure Solution, University of Göttingen, Göttingen, Germany, **1997**.

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3. L.J. Farrugia, J. Appl. Cryst. **1999,** *32*, 837-838.

4. L.J. Farrugia, J. Appl. Cryst. **1997**, *30*, 565.