Supplementary Material (ESI) for PCCP

1-Alkyl-3-methylimidazolium alkanesulfonate ionic liquids, $[C_nH_{2n+1}mim][C_kH_{2k+1}SO_3]$: synthesis and physicochemical properties

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ELECTRONIC SUPPORTING INFORMATION

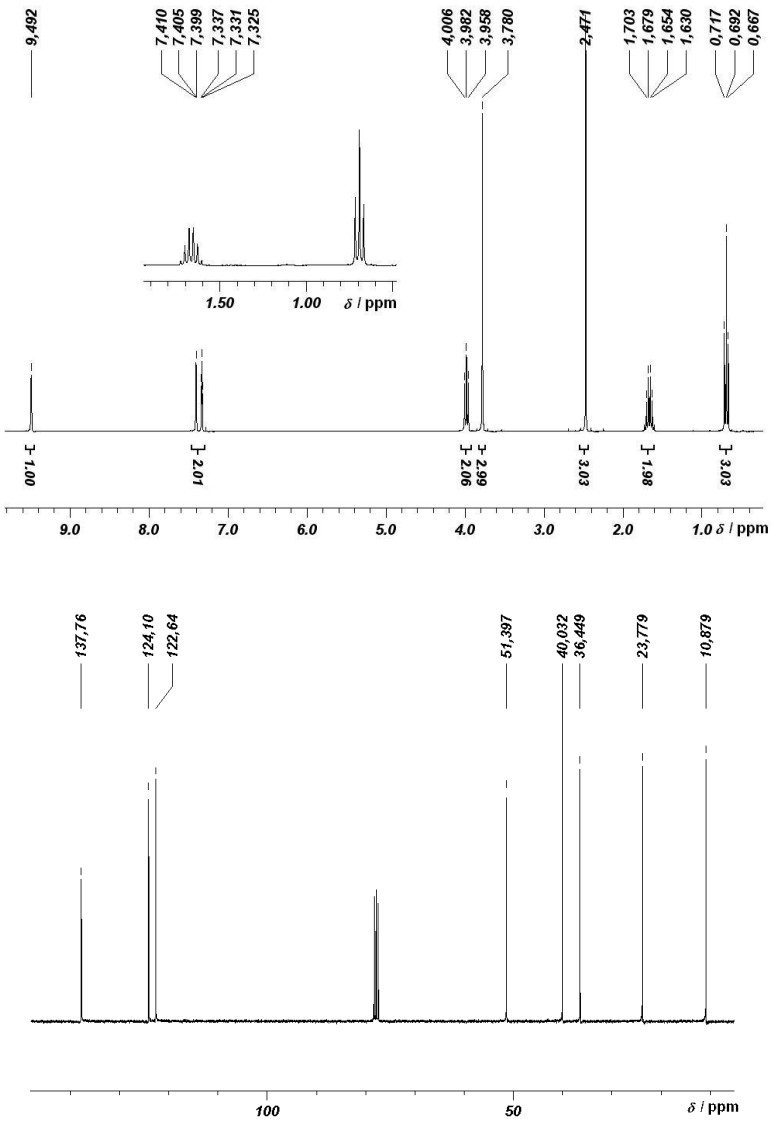

Figure 1S. Typical examples of the NMR spectra of $[C_n\text{mim}][C_kSO_3]$ ionic liquids; the ^{1}H NMR spectrum (300 MHz, 27 °C, $CDCl_3$), top, and the $^{13}C\{^1H\}$ NMR spectrum (75 MHz, 27 °C, $CDCl_3$), bottom, of $[C_3\text{mim}][SO_3CH_3]$

Table 1S ^{1}H NMR signals obtained for [$C_n$mim][C_kSO_3] ionic liquids (300 MHz, 27 °C, $CDCl_3$). In the case of ionic liquids with (n=1,k=1), (n=1,k=4) and (n=4, k=2) the data are comparable with the values reported in the ESI of ref. 5 of the present manuscript.

k	*n*	H(2)	H(5)	H(4)	NC*H*$_2$	NC*H*$_3$	SC*H*$_2$	SCH$_2$C*H*$_2$	S(CH$_2$)$_2$ C*H*$_2$	S(CH$_2$)$_3$ (C*H*$_2$)$_{k-3}$	S(CH$_2$)$_{k-1}$ C*H*$_3$	NCH$_2$C*H*$_2$	N(CH$_2$)$_2$ (C*H*$_2$)$_{n-3}$CH$_3$	(CH$_2$)$_{n-1}$ C*H*$_3$
1	**1**	9.70, s, 1H	7.61, s, 1H	7.61, s, 1H		4.03, s, 1H					2.75, s, 3H			4.03, s, 3H
	2	9.13, s, 1H	7.19, s, 1H	7.16, s, 1H	3.80, q, *J* = 7.5, 2H	3.50, s, 3H					2.15, s, 3H			1.0, t, *J* = 7.5, 3H
	3	9.49, s, 1H	7.41, d, *J* = 1.8, 1H	7.33, d, *J* = 1.8, 1H	3.98, t, *J* = 7.2, 2H	3.70, s, 3H					2.47, s, 3H	1.63-1.71, m, *J* = 7.5, 2H		0.69, t, *J* = 7.5, 3H
	4	9.81, s, 1H	7.66, s, 1H	7.55 (s) 1H	4.28, t, *J* = 7.2, 2H	4.06, s, 3H					2.47, s, 3H	1.84-1.94, m, *J* = 7.5, 2H	1.31-1.41, m, *J* = 7.5, 2H	0.99, t, *J* = 7.5, 3H
	5	9.81, s, 1H	7.66, d, *J* = 1.8, 1H	7.52, d, *J* = 1.8, 1H	4.27, t, *J* = 7.2, 2H	4.06, s, 3H					2.76, s, 3H	1.85-1.95, m, *J* = 7.5, 2H	1.28-1.40, m, *J* = 7.5, 4H	0.89, t, *J* = 6.8, 3H
	6	9.25, s, 1H	7.29, d, *J* = 1.5, 1H	7.18, d, *J* = 1.5, 1H	3.81, t, *J* = 6.3, 2H	3.61, s, 3H					2.76, s, 3H	1.32-1.53, m, *J* = 7.5, 2H	0.80-1.0, m, *J* = 7.5, 6H	0.41, t, *J* = 6.8, 3H
	8	9.48, s, 1H	7.41, *J* = 1.5, 1H	7.27, d, *J* = 1.5, 1H	3.98, t, *J* = 6.9, 2H	3.70, s, 3H					2.46 s, 3H	1.53-1.63, m, *J* = 7.5, 2H	0.91-1.05, m, *J* = 7.5, 10H	0.56, t, *J* = 6.8, 3H
	10	9.68, s, 1H	7.61, s, 1H	7.45, s, 1H	4.18, t, *J* = 7.5, 2H	3.97, s, 3H					2.67, s, 3H	1.72-1.84, m, *J* = 6.6, 2H	0.90-1.18, m, *J* = 7.5, 14H	0.79, t, *J* = 6.6, 3H
2	**2**	9.48, s, 1H	7.35, s, 1H	7.34, s, 1H	4.02, t, *J* = 7.5, 2H	3.72, s, 3H	2.50, q, *J* = 7.5, 2H				1.32, s, 3H,			0.99, t, *J* = 7.5, 3H
	3	9.85, s, 1H	7.69, d, *J* = 6.6, 1H	7.60, d, *J* = 6.6, 1H	4.26, t, *J* = 7.2, 2H	4.06, s, 3H	2.85, q, *J* = 7.5, 2H				1.34, t, *J* = 7.5, 3H	1.90-2.05, m, *J* = 7.5, 2H		0.97, t, *J* = 7.5, 3H
	4	10.06, s, 1H	7.39, d, *J* = 1.8, 1H	7.28, d, *J* = 1.8 1H	4.28, t, *J* = 7.5, 2H	4.06, s, 3H	2.89, q, *J* = 7.5, 2H				1.26-1.33, m, *J* = 7.5, 3H	1.88, m, *J* = 7.5, 2H	1.26-1.33, m, *J* = 7.5, 2H	0.96, t, *J* = 7.2, 3H
	5	10.02, s, 1H	7.44, d, *J* = 1.8, 1H	7.32, d, *J* = 1.8, 1H	4.26, t, *J* = 7.5 2H	4.06, s, 3H	2.88, q, *J* = 7.5, 2H				1.28-1.37, m, *J* = 7.5, 3H	1.89, m, m, *J* = 7.5, 2H	1.28-1.37, m, *J* = 7.5, 4H	0.90, t, *J* = 6.9, 3H
	6	9.50, s, 1H	7.42, d, *J* = 1.8, 1H	7.27, d, *J* = 1.8, 1H	3.96, t, *J* = 7.5, 2H	3.74, s, 3H	2.50, q, *J* = 7.5, 2H				0.95-1.07, m, *J* = 7.5, 3H	1.57, m, *J* = 7.5, 2H	0.95-1.07, m, *J* = 7.5, 6H	0.55, t, *J* = 6.9, 3H
3	**2**	9.85, s, 1H	7.64, d, *J* = 1.8, 1H	7.62, d, *J* = 1.8, 1H	4.35, t, *J* = 7.5, 2H	4.05, s, 3H	2.80, q, *J* = 3.3, 2H	1.85, m, *J* = 7.5, 3H			1.57, t, *J* = 7.5, 3H			1.01, t, *J* = 7.5, 3H
	3	9.32, s, 1H	7.31, d, *J* = 1.5, 1H	7.25, d, *J* = 1.8, 1H	3.84, t, *J* = 7.5, 2H	3.63, s, 3H	2.35, t, *J* = 6.0, 2H	1.36-1.54, m, *J* = 7.2, 2H			0.50-0.60, m, *J* = 7.2, 3H	1.36-1.54, m, *J* = 7.2, 2H		0.50-0.60, m, *J* = 7.2, 3H
4	**2**	9.86, s, 1H	7.63, d, *J* = 1.5, 1H	7.61, d, *J* = 1.5, 1H	4.36, q, *J* = 7.5, 2H	4.05, s, 3H	2.80, t, *J* = 1.8, 2H	1.81, q, *J* = 1.5, 2H	1.37-1.49, m, *J* = 7.5, 2H		0.91, t, *J* = 7.2, 3H			1.57, t, *J* = 6.8, 3H
	3	9.87, s, 1H	7.65,d, *J* = 1.5 1H	7.55, d, *J* = 1.5, 1H	4.25, t, *J* = 7.2, 2H	4.05, s, 3H	2.83, t, *J* = 6.5, 2H	1.76-1.84, m, *J* = 7.5, 2H	1.36-1.49, m, *J* = 7.5, 2H		0.89-0.99, m, *J* = 7.5, 3H	1.76-1.84, m, *J* = 7.5, 2H		0.89-0.99, m, *J* = 7.5, 3H
6	**2**	9.55, s, 1H	7.39, s, 1H	7.34, s, 1H	4.03, t, *J* = 7.2, 2H	3.76, s, 3H	2.48, t, *J* = 7.8, 2H	1.43-1.51, m, *J* = 7.5, 2H	1.02-1.09, m, *J* = 7.2, 2H	0.94-0.97, m, *J* = 7.2, 4H	0.54, t, *J* = 6.6, 3H			1.24, m, *J* = 7.5, 3H

Table 2S $^{13}C\{^{1}H\}$ NMR signals obtained for $[C_n mim][C_k SO_3]$ ionic liquids (75 MHz, 27 °C, $CDCl_3$). In the case of ionic liquids with (n=1, k=1), (n=1, k=4) and (n=4, k=2) the data are comparable with the values reported in the ESI of ref. 5 of the present manuscript.

k	*n*	C2	C5	C4	N*C*H$_2$	N*C*H$_3$	S*C*H$_2$	SCH$_2$*C*H$_2$	S(CH$_2$)$_2$*C*H$_2$	S(CH$_2$)$_3$(*C*H$_2$)$_{k-3}$	S(CH$_2$)$_{k-1}$*C*H$_3$	NCH$_2$*C*H$_2$	N(CH$_2$)$_2$(*C*H$_2$)$_{n-3}$CH$_3$	(CH$_2$)$_{n-1}$*C*H$_3$
1	**1**	138.89	124.0	124.0		40.13					36.50			40.13
	2	131.81	124.03	122.12	44.39	44.13					36.01			10.01
	3	137.76	124.10	122.64	51.40	40.03					36.45	23.78		10.88
	4	137.88	124.17	122.56	49.80	40.05					36.51	32.35	19.63	13.65
	5	137.98	124.20	122.49	50.11	40.08					36.57	30.19	28.49 22.29	14.09
	6	137.39	124.01	122.48	49.71	39.84					36.19	31.02	30.19 25.77 22.31	13.92
	8	137.74	124.18	122.67	49.99	39.98					36.42	31.79	30.47 29.15 29.08 26.36 22.69	14.21
	10	137.80	124.22	122.48	50.05	40.00					36.40	31.99	30.49 29.63 29.56 29.40 29.19 26.43 22.81	14.29
2	**2**	137.35	124.02	122.35	45.99	45.01	36.30				15.75			10.06
	3	137.94	124.16	122.63	51.44	46.15	36.50				10.92	23.85		10.19
	4	139.11	123.66	121.96	51.19	46.27	36.89				13.82	32.52	19.87	10.32
	5	137.52	123.98	122.59	50.06	46.20	36.42				14.02	31.88	29.89 25.62	10.19
	6	137.80	124.18	122.48	49.94	46.06	36.39				14.06	31.21	30.38 29.97 22.49	10.11
3	**2**	137.71	124.12	122.36	54.36	42.22	36.50	19.19			15.88			13.80
	3	137.55	124.03	122.61	54.15	51.16	36.27	18.96			13.66	23.67		10.71
4	**2**	138.45	123.13	121.40	51.15	44.16	35.46	26.71	21.28		14.87			13.08
	3	138.16	124.16	122.60	52.27	51.53	36.59	27.83	22.42		14.16	23.91		10.98
6	**2**	137.48	124.05	122.34	52.43	45.08	36.38	31.72	28.75	25.58 22.58	15.81			14.18