

Supporting Information

For

Measurement and Correlation of Solubility of Benzothiazolium Ionic Liquids in Ethanol + Ethyl Benzoate

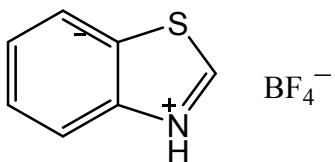
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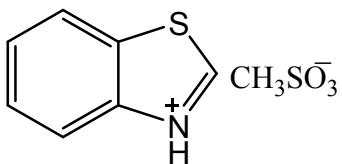
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Spectral data of the synthesized ILs

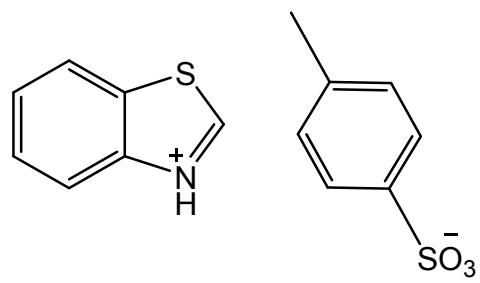
Benzothiazolium tetrafluoroborate ([HBth]/[BF₄]). Yield: 95 %. **¹H-NMR** (400 MHz, DMSO-d₆): δ, 9.51-9.23 (m, 2H), 8.18 (q, J = 8.0 Hz, 2H), 7.62-7.52 (m, 2H). **¹³C-NMR** (100 MHz, DMSO-d₆): δ 156.4, 152.4, 133.3, 126.3, 125.6, 122.7, 122.5. **MS** (ESI+) Calcd. For C₇H₆NS⁺: 136.0, Found: m/z 136.1; **MS** (ESI-) Calcd. For BF₄⁻: 87.0, Found: m/z 87.1.



Benzothiazolium methanesulfonate ([HBth]/[CH₃SO₃]). Yield: 96 %. **¹H-NMR** (400 MHz, DMSO-d₆): δ 89.50 (s, 1H), 9.08 (s, 1H), 8.18 (q, J=8.0 Hz, 2H), 7.61-7.1 (m, 2H), 2.62 (s, 3H). **¹³C-NMR** (100 MHz, DMSO-d₆): δ 156.4, 152.4, 133.4, 126.3, 125.5, 122.8, 122.5, 38.1. **MS** (ESI+) Calcd. For C₇H₆NS⁺: 136.0, Found: m/z 136.2; **MS** (ESI-) Calcd. For CH₃O₃S⁻: 95.0, Found: m/z 95.1.



Benzothiazolium p-toluenesulfonate ([HBth]/[p-TSA]). Yield: 96 %. **¹H-NMR** (400 MHz, DMSO-d₆): δ 12.01 (s, 1H), 9.52 (s, 1H), 8.17 (q, J=8.0 Hz, 2H), 7.61-7.50 (m, 4H), 7.19 (d, J=8.0 Hz, 2H), 2.31 (s, 3H). **¹³C-NMR** (100 MHz, DMSO-d₆): δ 156.5, 152.2, 144.3, 138.5, 133.4, 128.3, 126.3, 125.6, 125.5, 122.7, 122.6, 20.8. **MS** (ESI+) Calcd. For C₇H₆NS⁺: 136.0, Found: m/z 136.1; **MS** (ESI-) Calcd. For C₇H₇O₃S⁻: 171.0, Found: m/z 170.9.



Copies of ^1H NMR and ^{13}C NMR spectra:

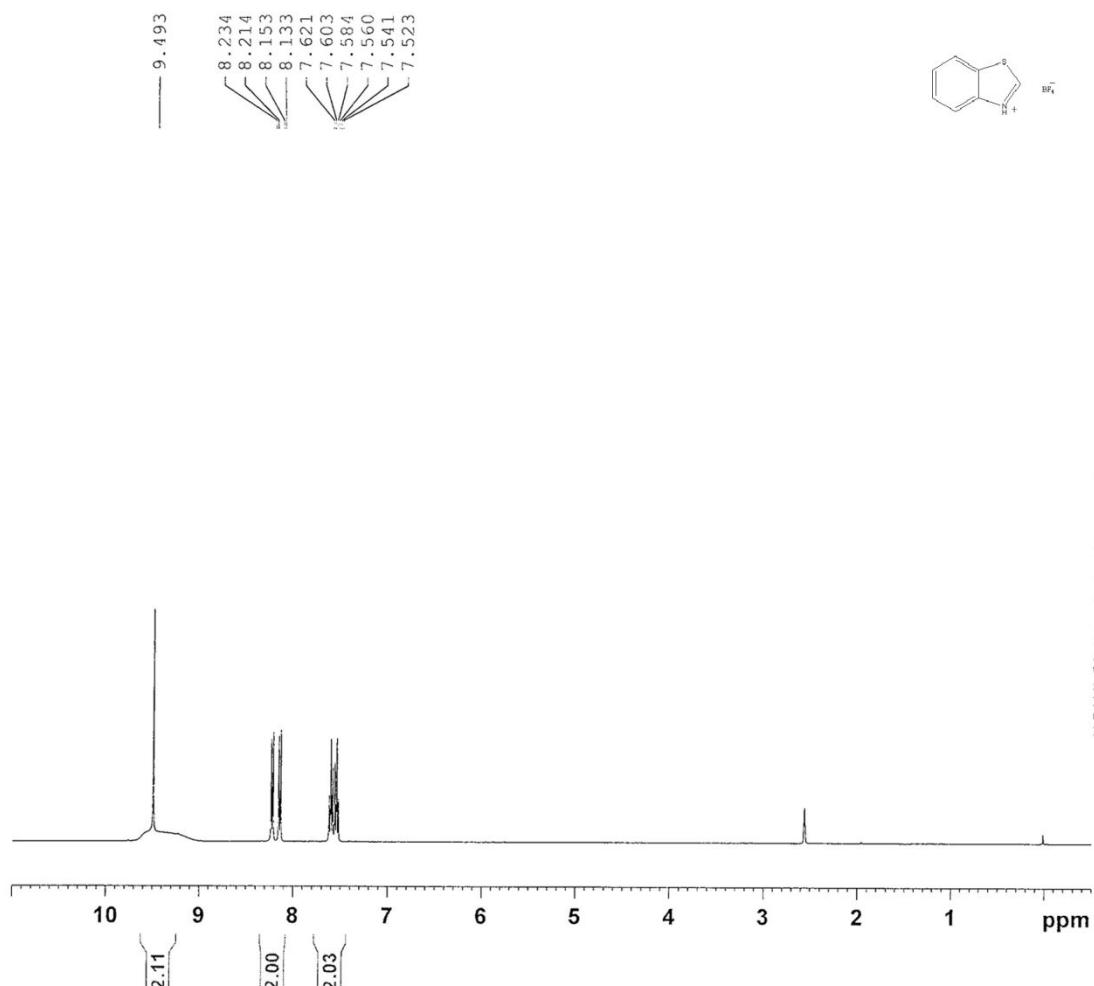


Figure S1 ^1H NMR spectrum of $[\text{HBth}][\text{BF}_4]$

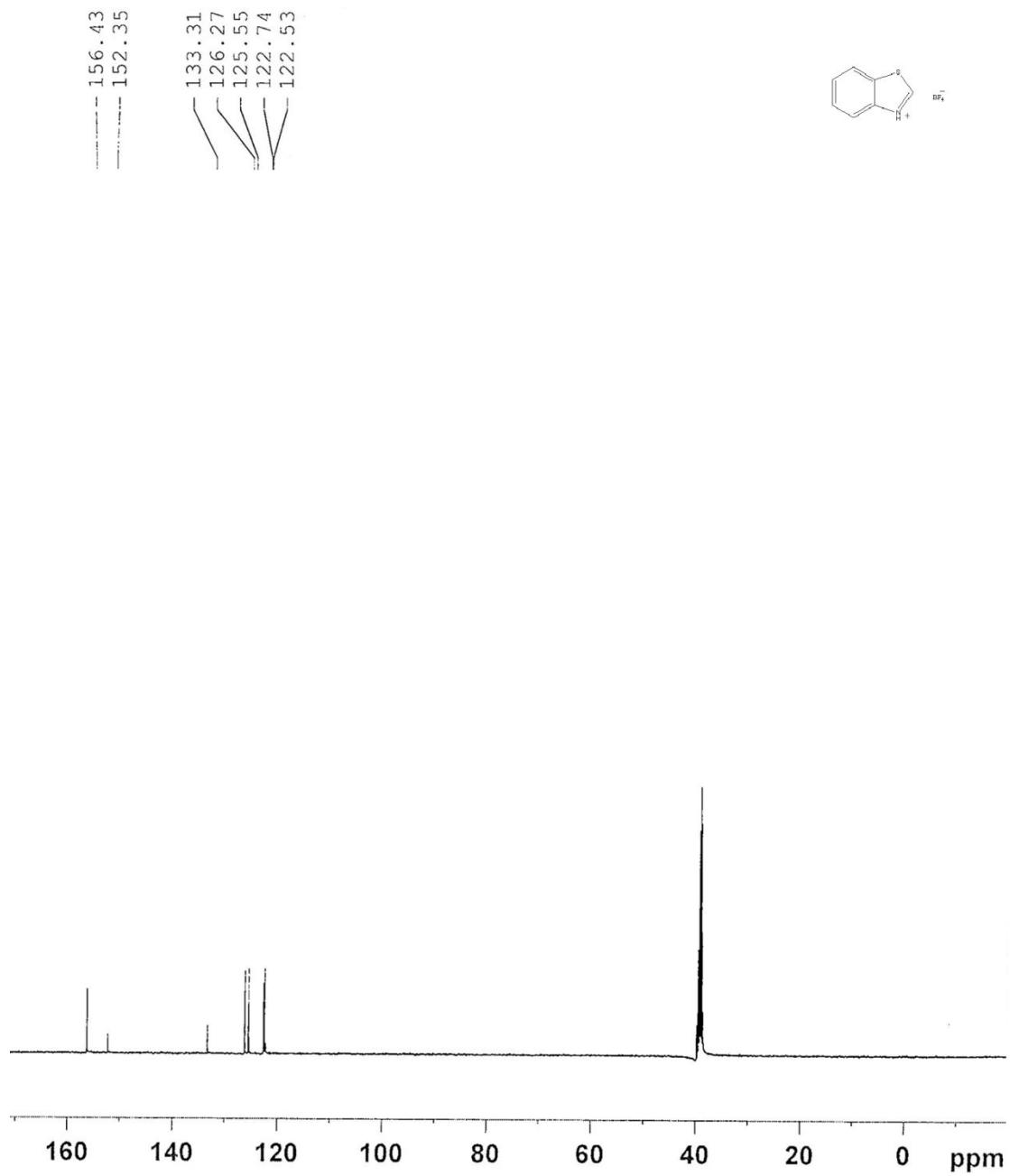


Figure S2 ^{13}C NMR spectrum of $[\text{HBth}][\text{BF}_4]$

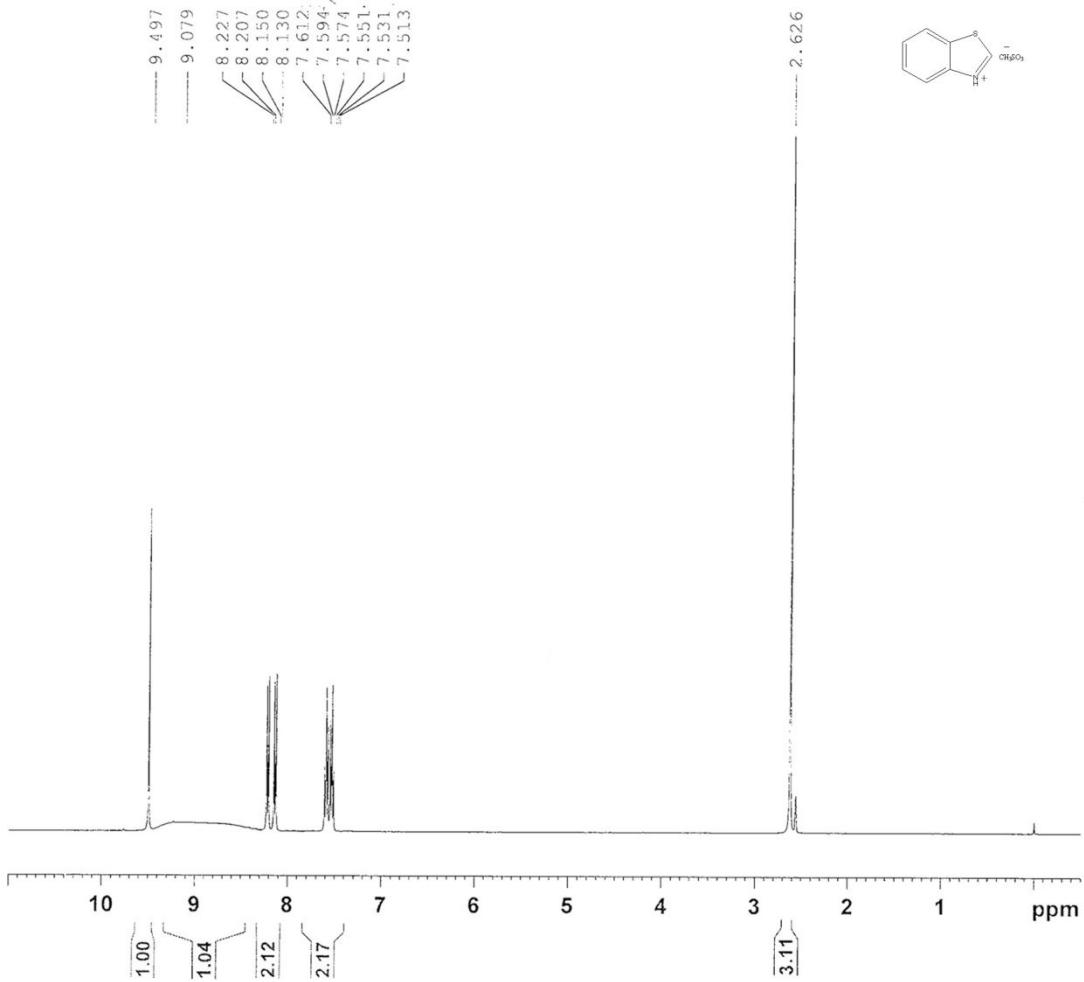


Figure S3 ¹H NMR spectrum of [HBth][CH₃SO₃]

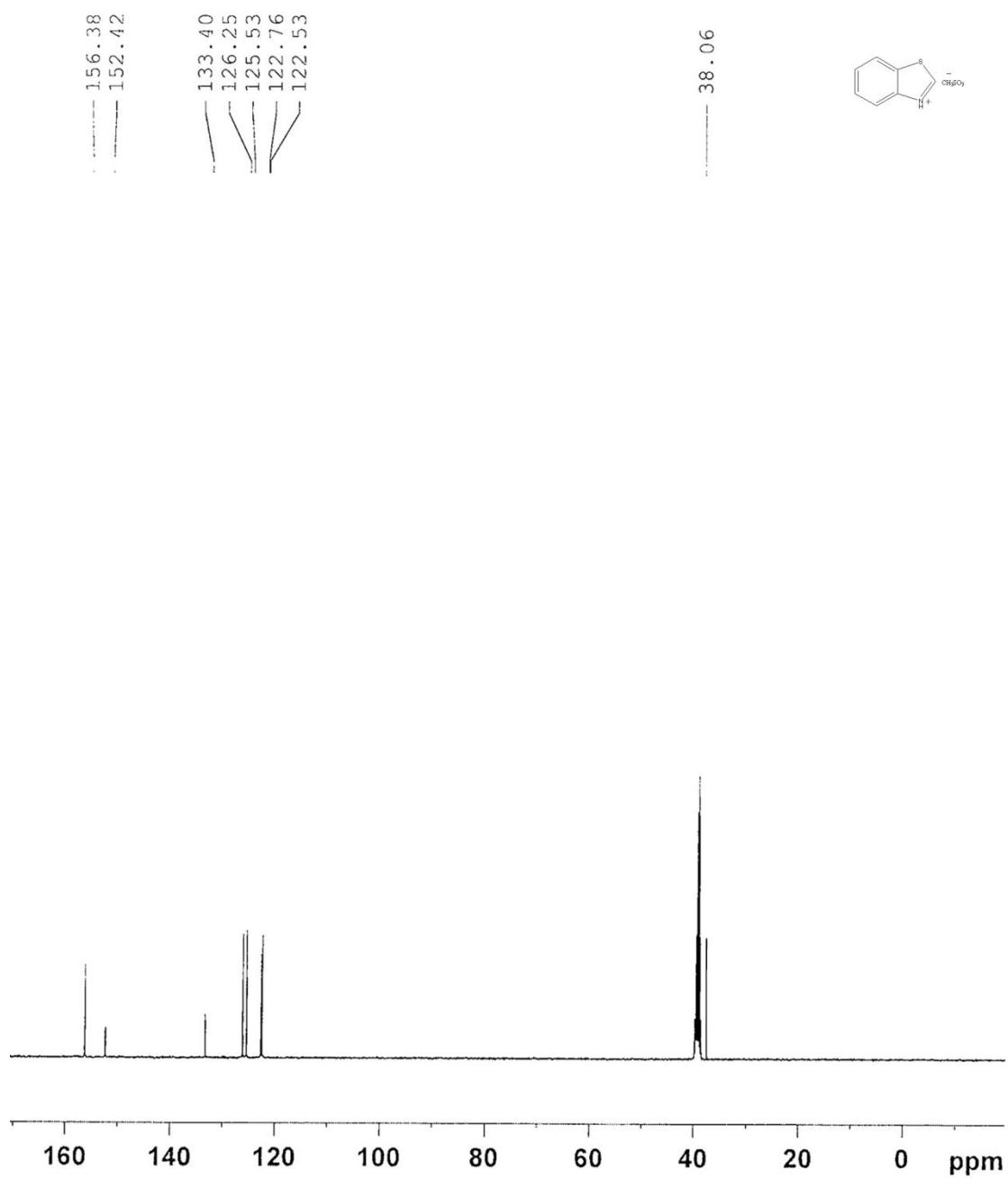


Figure S4 ¹³C NMR spectrum of [HBth][CH₃SO₃]

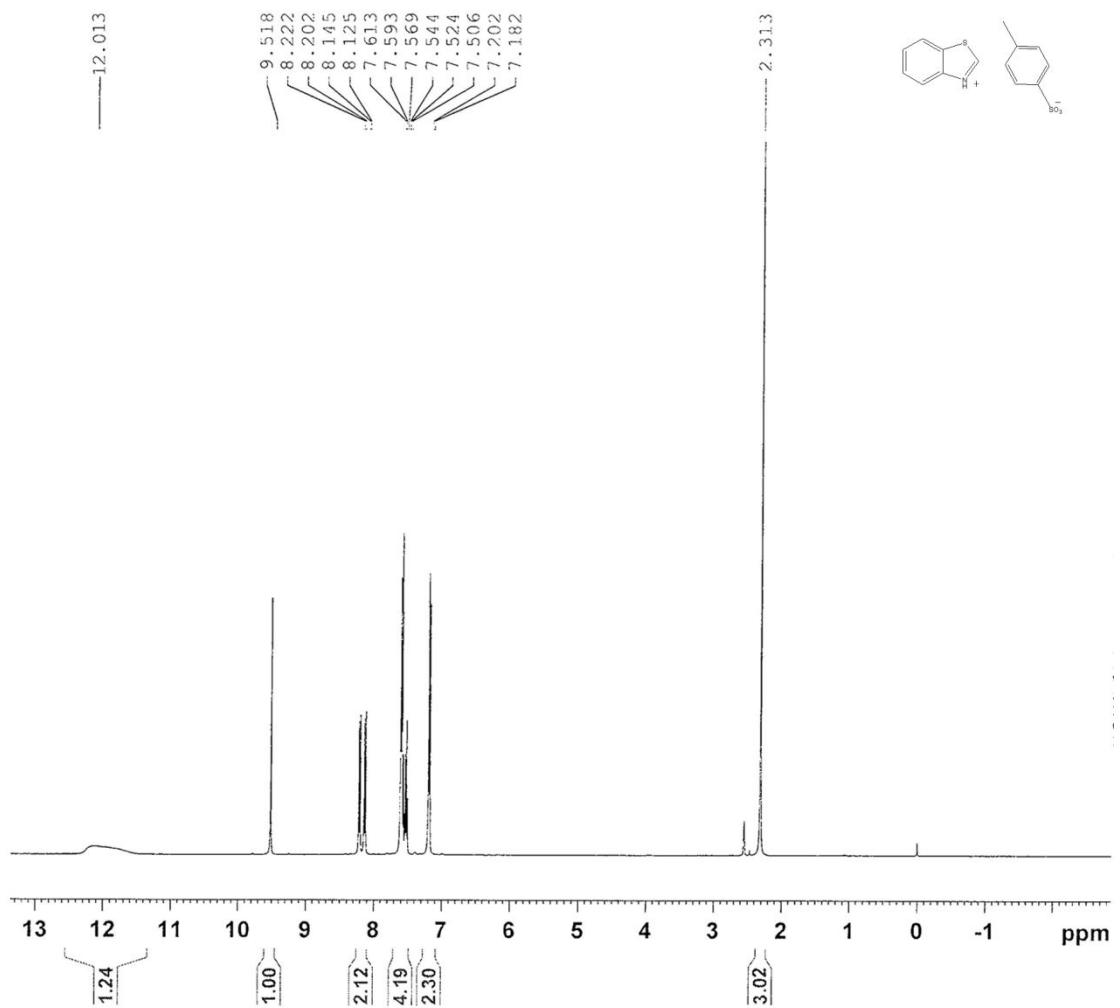


Figure S5 ¹H NMR spectrum of [HBth][p-TSA]

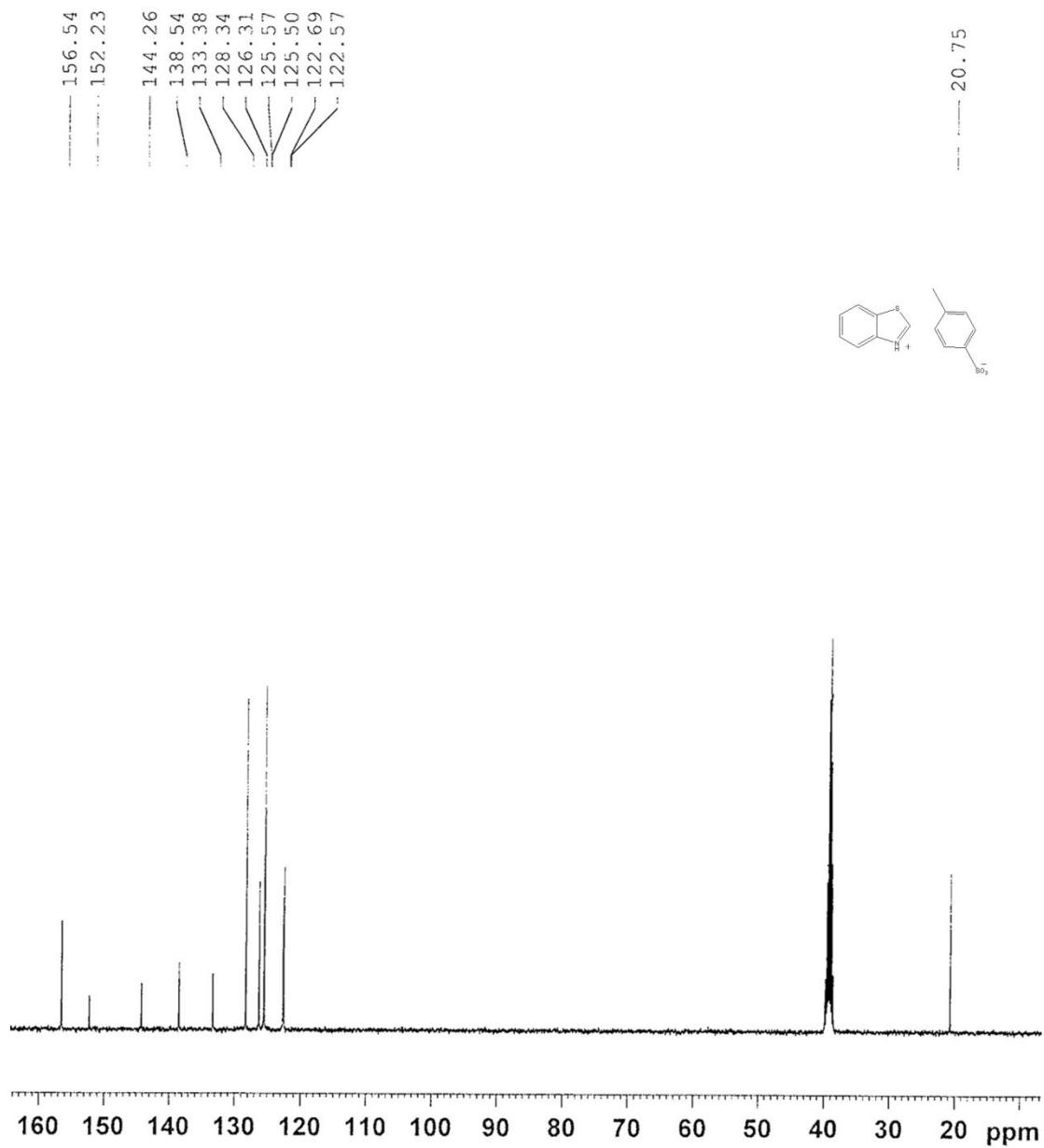


Figure S6 ^{13}C NMR spectrum of $[\text{HBth}][\text{p-TSA}]$

Comparison of solubility data in ethanol:

We carefully determined the solubilities of 3 ILs in ethanol and compared these results with Ref. 19 (J. Chem. Thermodyn. 2014, 48-53). The detailed results are listed as Table S1. It can be seen from this table that all measured solubility data were close to reported data in Ref. 19 and all their relative deviations were less than 2%.

Table S1. The comparison of 3 ILs` solubility data in ethanol of this work with Ref. 19.

<i>[HBth]/[BF₄]</i>														
This work	T/K	293.7	288.5	283.3	278.4	273.2	268.4	263.6	258.5	253.4	248.3	243.1	238.3	233.2
	x ^{exp} ×10 ³	13.79	11.17	9.241	7.714	6.659	5.718	4.986	4.431	4.01	3.679	3.420	3.295	3.249
Ref.19	T/K	293.85		283.05	278.15	273.25	268.15	263.35		253.15				
	X ^{exp} ×10 ³	13.9		9.27	7.70	6.68	5.83	5.06		4.08				
RD(%)														
0.791														
<i>[HBth]/[CH₃SO₃]</i>														
This work	T/K	293.7	288.5	283.3	278.4	273.2	268.4	263.6	258.5	253.4	248.3	243.1	238.3	233.2
	x ^{exp} ×10 ³	9.724	7.697	6.175	5.270	4.398	3.674	2.984	2.583	2.273	1.978	1.781	1.627	1.510
Ref.19	T/K	293.85		283.05	278.15	273.25	268.15	263.35		253.15				
	X ^{exp} ×10 ³	9.82		6.28	5.22	4.41	3.69	3.03		2.30				
RD(%)														
0.978														
<i>[HBth]/[p-TSA]</i>														
This work	T/K	293.7	288.5	283.3	278.4	273.2	268.4	263.6	258.5	253.4	248.3	243.1	238.3	233.2
	x ^{exp} ×10 ³	11.80	9.706	7.917	6.312	5.029	4.271	3.566	3.068	2.677	2.224	1.928	1.685	1.493
Ref.19	T/K	293.85		283.05	278.15	273.25	268.15	263.35		253.15				

X ^{exp} ×10 ³	11.6	7.86	6.36	4.97	4.34	3.59	2.72
RD(%)	1.724	0.725	0.755	1.187	1.590	0.669	1.581
