SUPPORTING INFORMATION

CO_2 Capture Efficiency, Corrosion Properties and Ecotoxicity Evaluation of Amine Solutions Involving Newly Synthesized Ionic Liquids

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1. Assumptions made for the derivation of the solution of the transient absorption equation.

(1) Gas dissolves through a one-dimensional (vertical) diffusion process, in which there is no convective flow in the liquid.

(2) A thin boundary layer between the gas and liquid phases exists, where the thermodynamic equilibrium is instantly established with the saturation concentration and where the concentration is constant all the time at a given temperature and pressure.

(3) Temperature and pressure are kept constant.

(4) The uptake occurs over a small change in the absorbed phase concentration and thereby constant diffusivity is assumed.

(5) The uptake within the absorbent sample is very small compared to the capacity of the system, which is implicitly valid in the Henry's law regime, i.e. for a very dilute absorbed phase.

Table S1: The chemical structures of the ILs examined in this work.

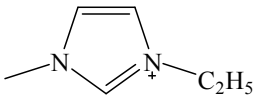
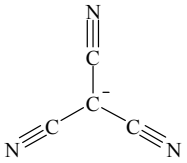
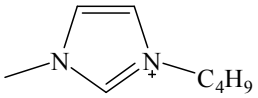
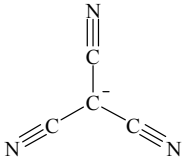
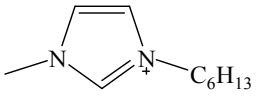
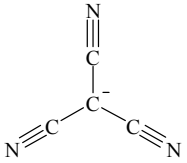
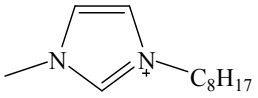
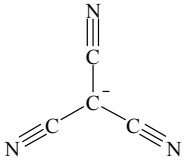
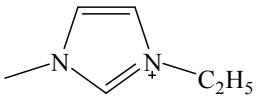
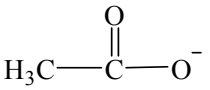
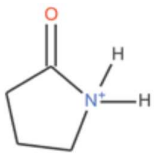
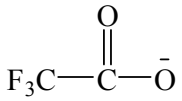
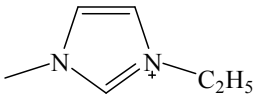
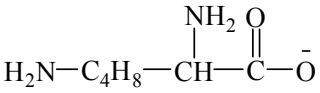
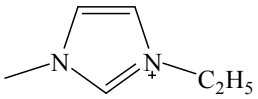
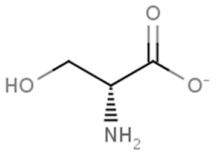
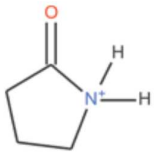
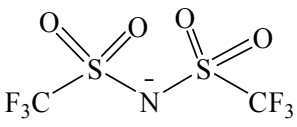
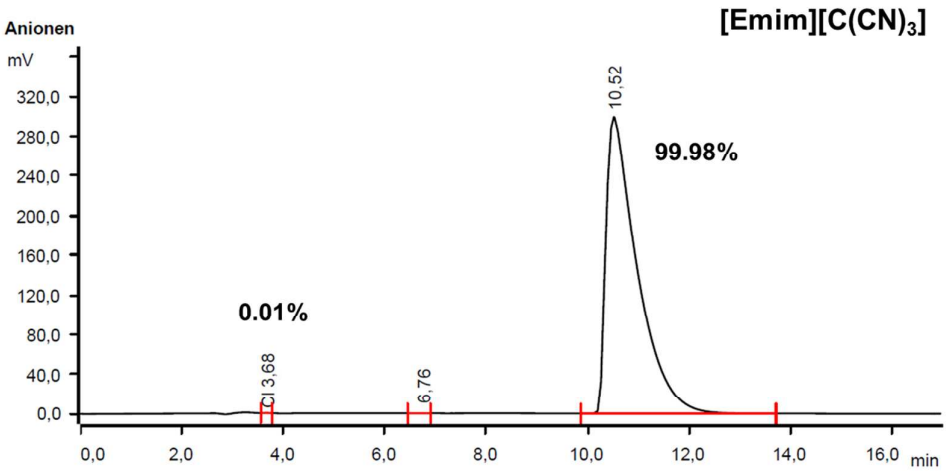
	Cation	Anion
1-ethyl-3-methyl-imidazolium tricyanomethanide		
1-butyl-3-methyl-imidazolium tricyanomethanide		
1-hexyl-3-methyl-imidazolium tricyanomethanide		
1-octyl-3-methyl-imidazolium tricyanomethanide		
1-ethyl-3-methyl-imidazolium acetate		
Pyrrolidium-2-one trifluoroacetate		
1-ethyl-3-methyl-imidazolium lysinate		
1-ethyl-3-methyl-imidazolium serinate		
Pyrrolidium-2-one bis(trifluoromethylsulfonyl)imide		

Table S1: Ion purity, water content and halides content in the IL samples examined.

Ionic Liquid	Assay NMR	Water content (%)	Anion (IC*)	Cation (IC)	Halides (IC)
1-ethyl-3-methyl-imidazolium tricyanomethanide	>98%	0.093	99.9%	99.7 %	<0.5%
1-butyl-3-methyl-imidazolium tricyanomethanide	>98%	0.072	99.8%	98.9%	<0.5%
1-hexyl-3-methyl-imidazolium tricyanomethanide	>98%	0.039	99.9%	99.8%	<0.5%
1-octyl-3-methyl-imidazolium tricyanomethanide	>98%	0.012	99.9%	99.5%	<0.5%
1-ethyl-3-methyl-imidazolium acetate	>95%	0.385	99.6 %	99.7 %	<0.1%
Pyrrolidium-2-one trifluoroacetate	>98%	0.082	>98%	>98%	<0.1%
1-ethyl-3-methyl-imidazolium lysinate	>98%	1.355	-	-	-
1-ethyl-3-methyl-imidazolium serinate	>98%	1.084	-	-	-
Pyrrolidium-2-one bis(trifluoromethylsulfonyl)imide	>98%	0.080	>98%	>98%	<0.5%

*Ion Chromatography

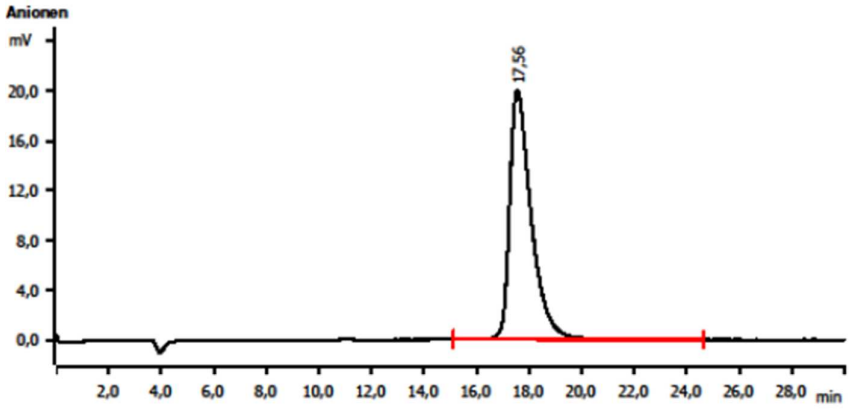
Figure S1: (a) Ion Chromatogram (anion) of [EMIM][TCM] showing chlorine content of 0.01%. (b) Ion chromatogram (anion) of [HMIM][TCM]. (c) Ion chromatogram (cation) of [HMIM][TCM].



(a)

Sample data

Ident	HMIM TCM r, JK
Measured by	IOLITEC
Determination start	2013-08-12 12:19:45 UTC+2
Info	Anionen
Info	ma-a2
Säule	Anionen - Neue Säule + Eluent 1



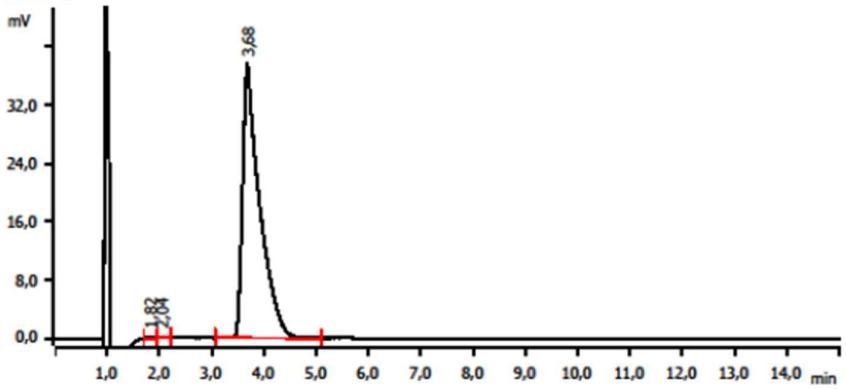
Peak number	Retention time min	Area (mV) x min	Height mV	Concentration mg/L	Area ratio %	Component name
1	17,555	19,1284	20,025	invalid	100,000	

(b)

Sample data

Ident ..... HMIM TCM, JK
Measured by ..... IOLITEC
Determination start ..... 2013-08-20 23:05:37 UTC+2
Info ..... Kationen
Info bb-k12
Säule ..... Kationen- mittellange Säule mit neuer

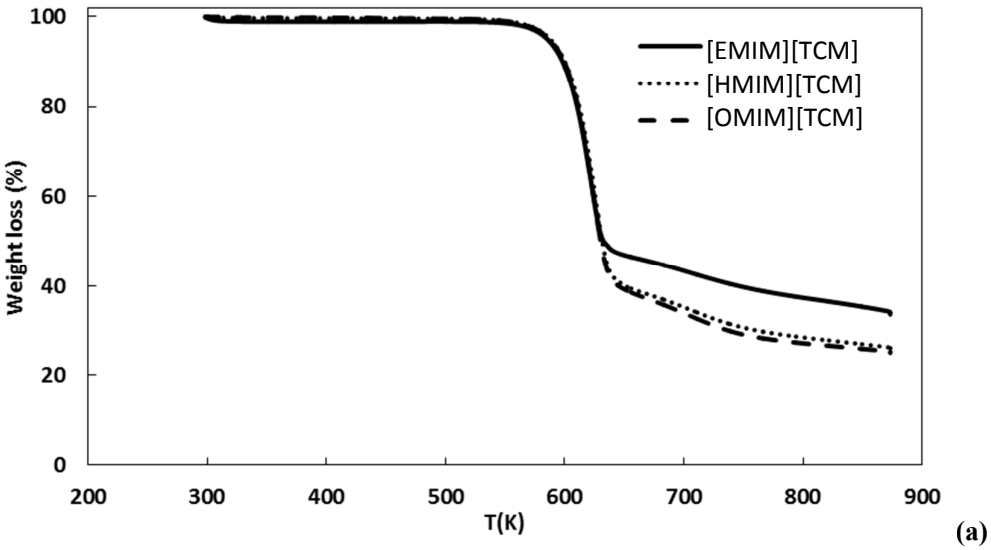
Kationen



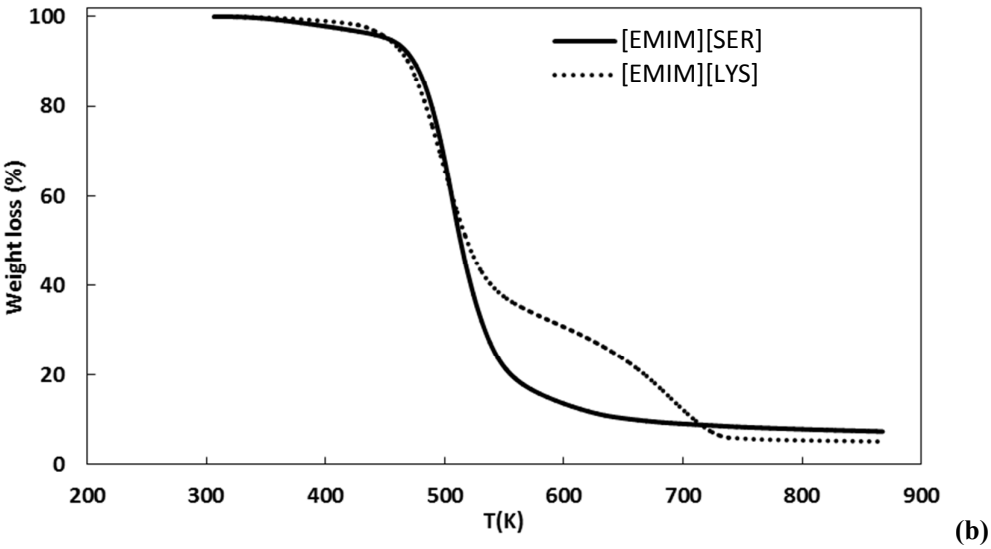
Peak number	Retention time	Area	Height	Concentration	Area ratio	Component name
	min	(mV) x min	mV	mg/L	%	
1	1,823	0,0123	0,071	invalid	0,087	
2	2,038	0,0084	0,051	invalid	0,059	
3	3,680	14,1517	37,497	invalid	99,854	

(c)

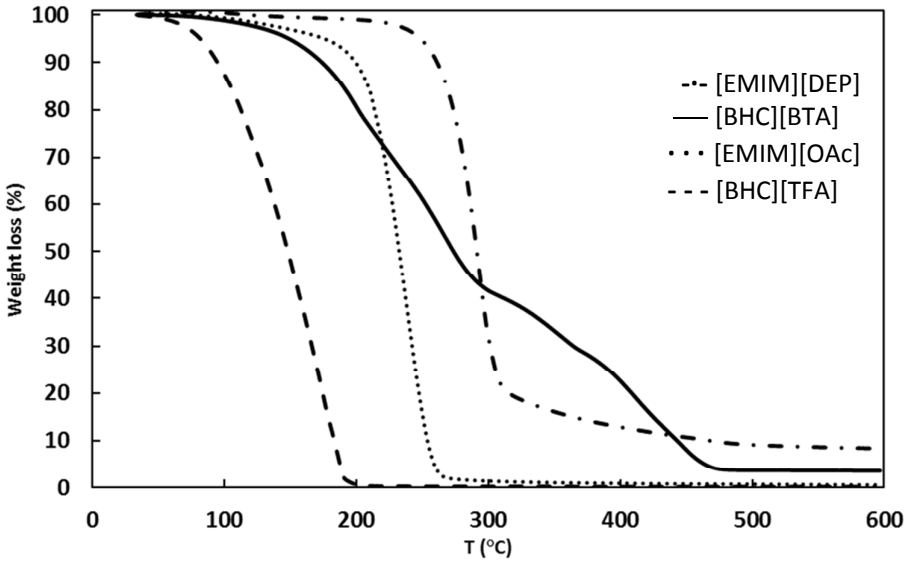
Figure S2: Dynamic TGA analysis of the ILs examined in this work and the respective derivatives. The analysis was carried out in a nitrogen environment and the temperature was raised by 5 ^{o}C/min. The thermographs show that the [TCM] anion based ILs exhibit the highest thermal stability (above 300^{o}C) whereas the aminoacid anion based ILs ([EMIM][LYS] and [EMIM][SER]) start to decompose at around 200^{o}C. The [BHC][BTA] presented two degradation stages with the first one occurring at 157^{o}C. The thermal degradation of [EMIM][OAc] started at 203^{o}C whereas the [BHC][TFA] had lost significant amount of mass from 100^{o}C which is attributed to evaporation.



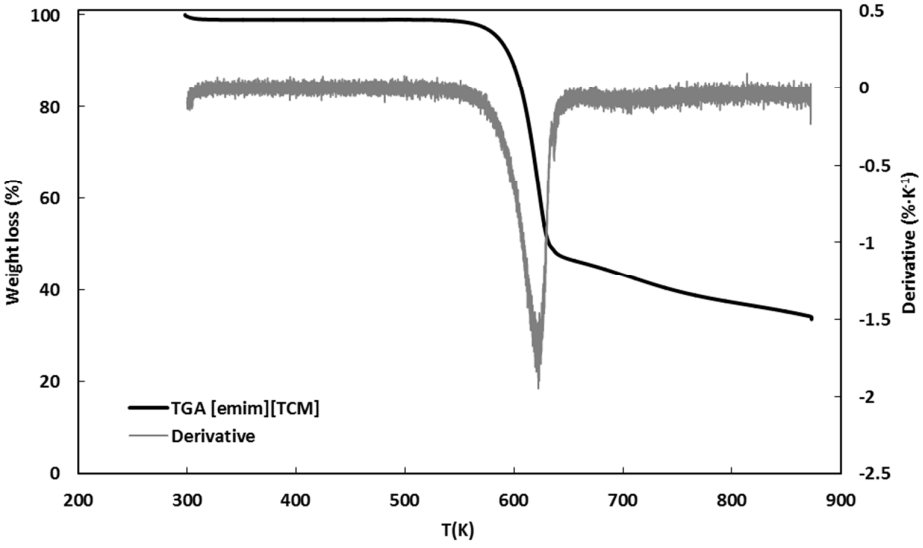
(a)



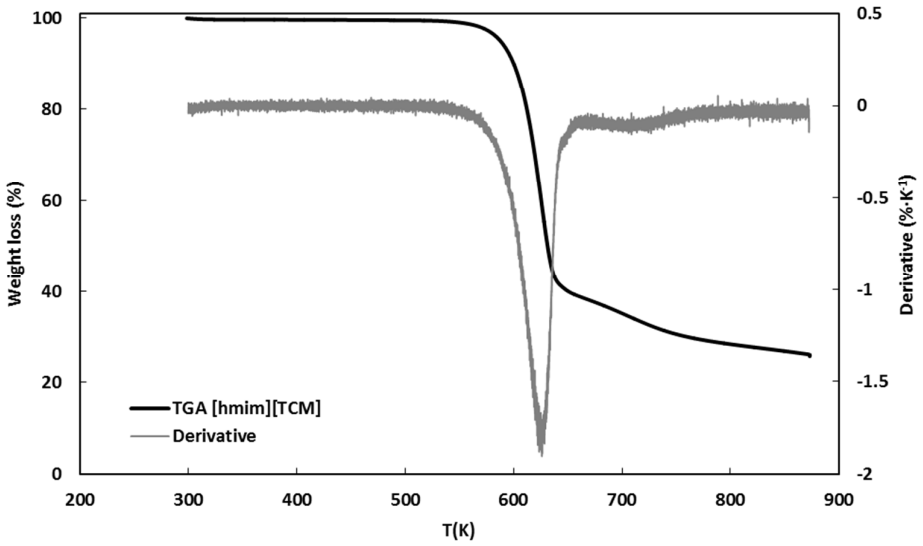
(b)


Weight loss (%)
T (°C)
[EMIM][DEP]
[BHC][BTA]
[EMIM][OAc]
[BHC][TFA]

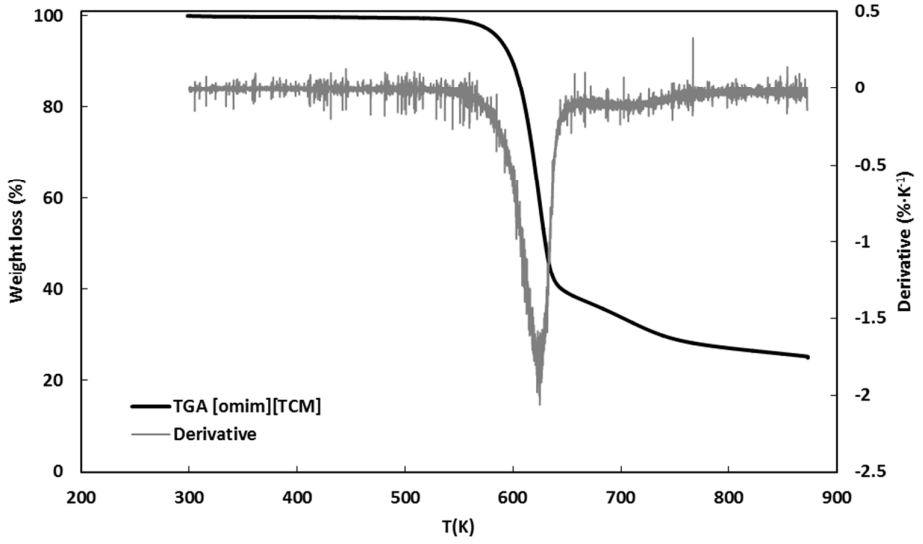
(c)


Weight loss (%)
Derivative (%·K-1)
T(K)
TGA [emim][TCM]
Derivative

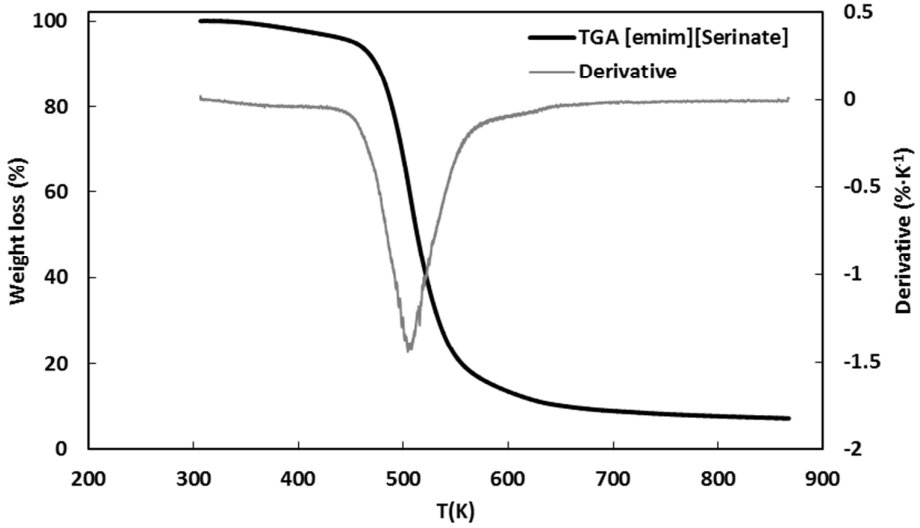
(d)


Weight loss (%)
Derivative (%·K-1)
T(K)
TGA [hmim][TCM]
Derivative

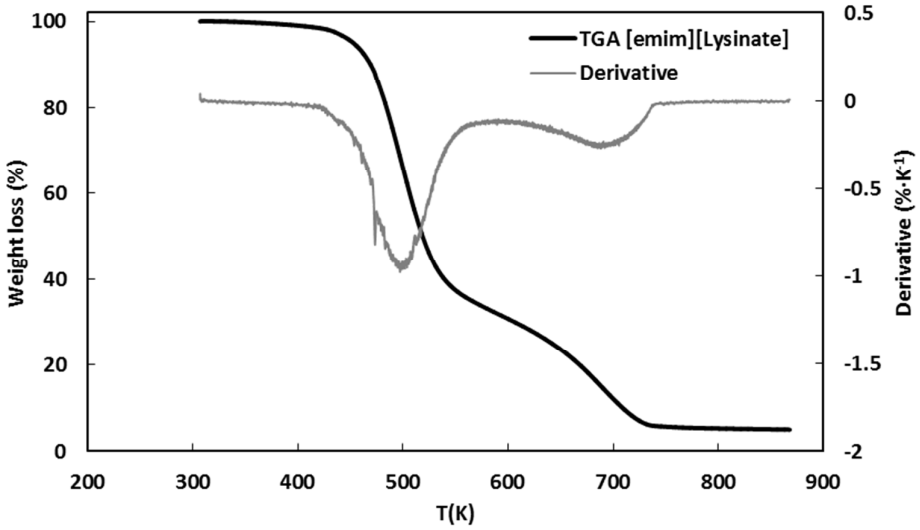
(e)


Weight loss (%)
Derivative (%·K-1)
T(K)
TGA [omim][TCM]
Derivative

(f)

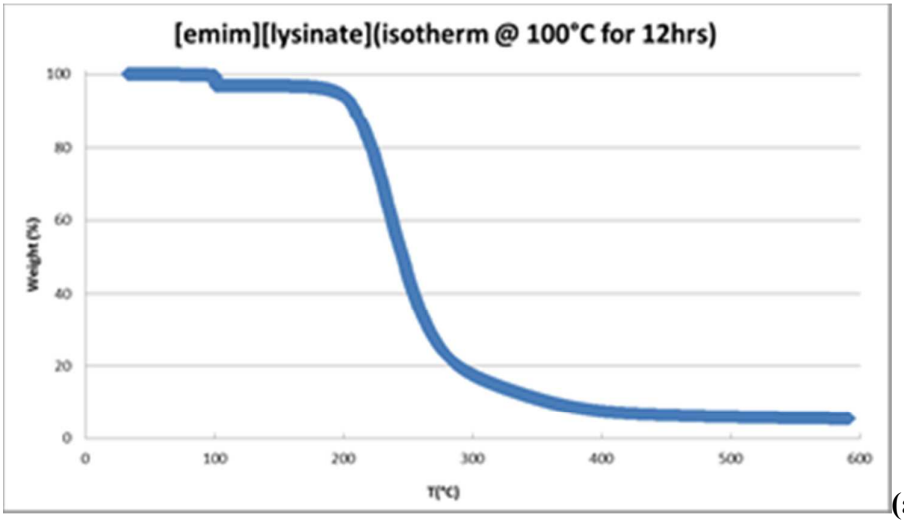

TGA [emim][Serinate]
Derivative
Weight loss (%)
Derivative (%·K-1)
T(K)
100
80
60
40
20
0
0.5
0
-0.5
-1
-1.5
-2
200
300
400
500
600
700
800
900

(g)

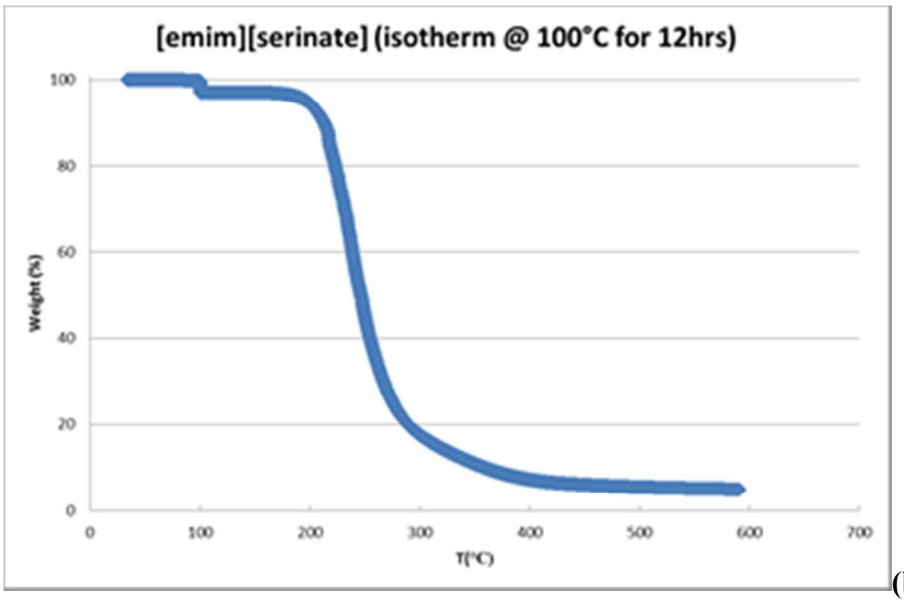

TGA [emim][Lysinate]
Derivative
Weight loss (%)
Derivative (%·K-1)
T(K)
100
80
60
40
20
0
0.5
0
-0.5
-1
-1.5
-2
200
300
400
500
600
700
800
900

(h)

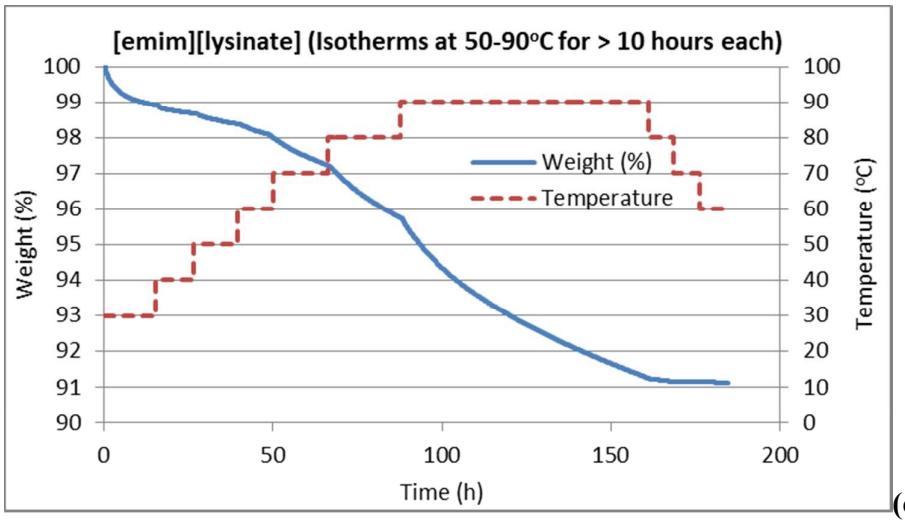
Figure S3: Isothermal TGA analysis of the aminoacid anion based ILs examined in this work. In thermographs (a, b) the analysis is carried out in a nitrogen environment and the temperature was raised by 5 ^{o}C/min. Both thermographs included an isothermal step at 100^{o}C for 12 hours where the two ionic liquids had lost 3% of their weight when the water content is 1.4 wt% and 1.7 wt% for [EMM][SER] and [EMIM][LYS] respectively. At 150^{o}C isotherm they showed a clear decomposition (the thermograph is not included). Because of the high water content of the [EMIM][LYS] and in order to accurately define the onset of its decomposition we performed a more detailed and longer thermal analysis and the results are presented in thermograph (c). The analysis was carried out under high vacuum (10^{-4} mbar) and the temperature was raised by 10^{o}C every 10-15 hours. It can be seen that the rate of mass loss becomes significant above 70^{o}C. From the thermograph it can be deduced that the onset of [EMIM][LYS] decomposition is somewhere between 80 and 90^{o}C in good accordance with the continuous degradation of the CO_2 capture performance of the solvent composed of [EMIM][LYS], [EMIM][SER] and water which was regenerated at 96^{o}C.



(a)


[emim][serinate] (isotherm @ 100°C for 12hrs)
Weight (%)
T(°C)
100
80
60
40
20
0
0
100
200
300
400
500
600
700

(b)


[emim][lysinate] (Isotherms at 50-90°C for > 10 hours each)
Weight (%)
Temperature (°C)
Time (h)
Weight (%)
Temperature
100
99
98
97
96
95
94
93
92
91
90
100
90
80
70
60
50
40
30
20
10
0
0
50
100
150
200

(c)

Figure S4: Macroscopic view of the MS specimens after treatment in (a) MIX B, (b) DEA 7%, MDEA 6.9%, (c) [EMIM][OAc] 20%.