New Hydrogen Carbonate Precursors for Efficient and Byproduct-Free Syntheses of Ionic Liquids Based on 1,2,3-Trimethylimidazolium and *N,N*-Dimethylpyrrolidinium Cores

Marcin Smiglak, C. Corey Hines,[1] and Robin D. Rogers[*]
Center for Green Manufacturing and Department of Chemistry, The University of Alabama, Tuscaloosa, AL 35487, USA

[1]Current Address: Nuclear Radiation Center, Washington State University, Pullman, WA 99164.

Table S1. NMR shifts of [1,2,3-triMeIM][$MeCO_3$] and [1,2,3-triMeIM][HCO_3] salts.

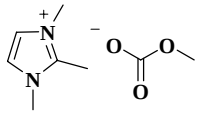
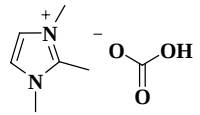
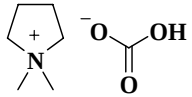
Sample Used	Entry	Solvent	Analyzed nuclei and time after dissolution	NMR shifts (ppm)							
				C2-$\underline{CH_3}$	N-$\underline{CH_3}$	C4/C5	$\underline{Me}CO_3$	MeOH	C2	$Me\underline{CO_3}$	$H\underline{CO_3}$
	**a**	$CDCl_3$	^{1}H after 10 min	2.74	3.94	7.74	3.45	trace @ 3.34	N/A	N/A	N/A
	b	$CDCl_3$	^{13}C after 10 min	9.52	35.16	122.69	52.02	---	143.99	157.98	---
	c	$CDCl_3$	^{1}H after 24 h	2.72 (H-D exchange)	3.94	7.71	3.45 (75%)	3.35 (25%)	N/A	N/A	N/A
	d	$CDCl_3$	^{13}C after 24 h	9.16	35.25	122.67	52.03	49.63	144.02	158.03	---
	e	D_2O	^{1}H after 10 min	2.58	3.78	7.30	3.54	3.37	N/A	N/A	N/A
	f	D_2O	^{1}H after 1 h	2.57	3.77	7.30	---	3.37	N/A	N/A	N/A
	g	D_2O	^{13}C after 1 h	9.30	35.21	122.43	---	49.58	145.39	---	160.94
	h	MeOD	^{1}H after 10 min	2.50	3.71	7.35	3.24	---	N/A	N/A	N/A
	i	MeOD	^{13}C after 10 min	9.34	35.42	123.35	49.90	---	146.52	161.37	---
	**j**	D_2O	^{1}H after 10 min	2.57	3.78	7.30	---	---	N/A	N/A	N/A
	k	D_2O	^{13}C after 10 min	9.41	35.32	122.55	---	---	145.50	---	161.03
	l	MeOD	^{1}H after 10 min	2.51	3.72	7.36	trace @ 3.24 (after 1 h)	---	N/A	N/A	N/A
	m	MeOD	^{13}C after 10 min	9.37	35.44	123.35	---	---	146.48	---	161.32

Table S2. NMR shifts of [*N*,*N*-diMePyr][HCO_3] salts.

Sample Used	Entry	Solvent	Analyzed nuclei and time after dissolution	NMR shifts (ppm)						
				CH_2-$\underline{CH_2}$	N-$\underline{CH_3}$	N-$\underline{CH_2}$	$\underline{Me}CO_3$	$\underline{Me}OH$	$MeCO_3$	HCO_3
	**a**	D_2O	^1H after 10 min	2.23	3.14	3.51	---	---	N/A	N/A
	b	D_2O	^{13}C after 10 min	21.65	51.67	65.82	---	---	---	160.17
	c	DMSO	^1H after 10 min	2.08	3.05	3.42	---	---	N/A	N/A
	d	DMSO	^{13}C after 10 min	21.76	51.50	65.33	---	---	---	158.93