Electronic Supplementary Information

First direct evidence of N-heterocyclic carbene in BMIm acetate ionic liquid. An electrochemical and chemical study on the role of temperature

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Content

Experimental Section

General remarks

All the ionic liquids were purchased from Iolitec and used after being kept at reduced pressure at room temperature for 24 h. Voltammetric measurements were performed using an Amel 552 potentiostat equipped with an Amel 566 function generator and an Amel 563 multipurpose unit in a three-electrode cell; the curves were displayed on an Amel 863 recorder; acquisition software was a CorrWare for windows version 2.8d1 Scribner, elaboration software was a CorrView for windows version 2.8d1 Scribner. A492/GC/3 Amel microelectrode was employed, using a Pt counter electrode and an Ag pseudoreference electrode. Mass spectra were recorded on a ThermoFinnigan LCQ Classic LC/MS/MS ion trap equipped with an ESI source and a syringe pump. Samples (10^{-4} - 10^{-5}M in MeOH/H_2O 90 : 10) were infused in the electrospray system at a flow rate of 5-10 µl min^{-1}.

Voltammograms

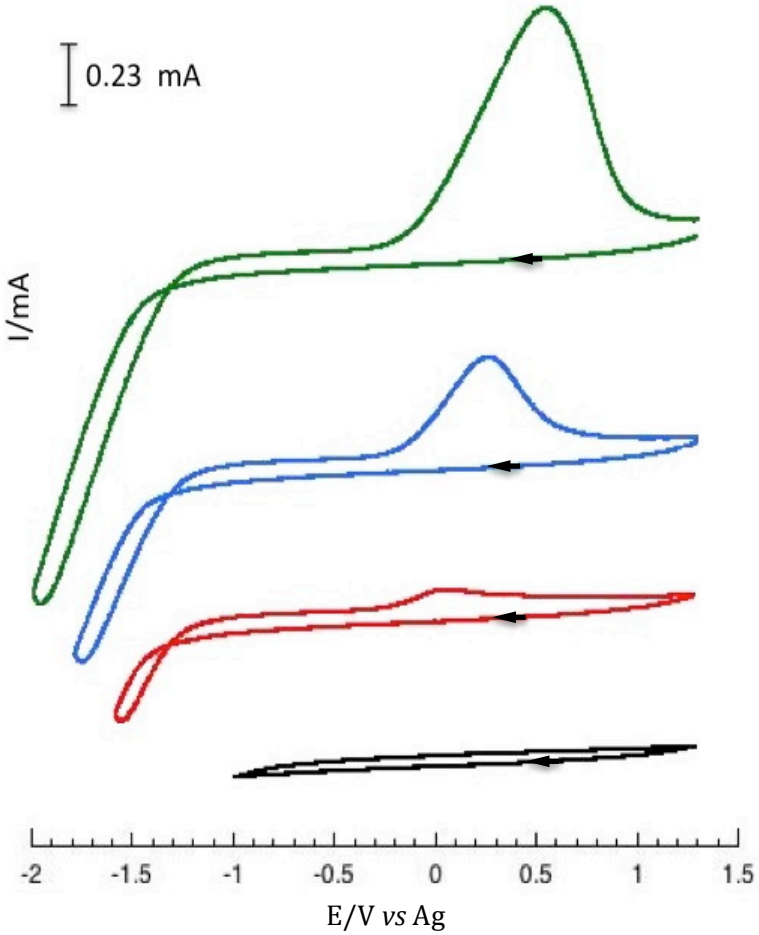

Figure S1 Cyclic voltammograms of BMImCl at 80°C. A492/GC/3 Amel microelectrode was employed, using a Pt wire counter electrode and an Ag wire pseudoreference electrode. The scanning rate was ν = 0.2 V s^{-1}. Scanning reversed at E = −1.0 V (black curve), E = −1.6 V (red curve), E = −1.8 V (blue curve), E = −2.0 V (green curve).

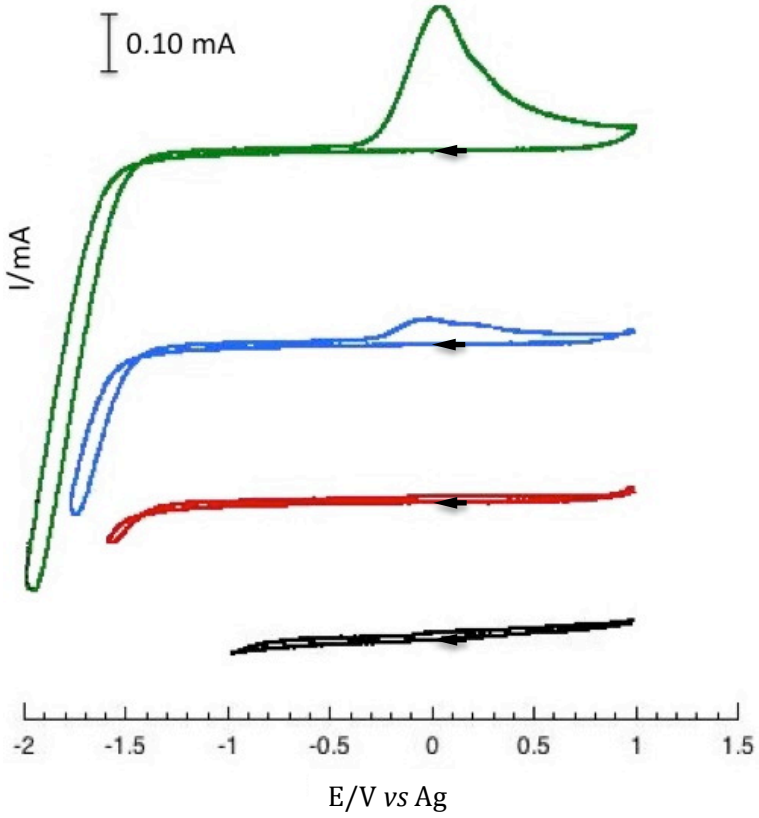

Figure S2 Cyclic voltammograms of BMImAcO at 80°C. A492/GC/3 Amel microelectrode was employed, using a Pt wire counter electrode and an Ag wire pseudoreference electrode.
The scanning rate was ν = 0.2 V s^{-1}. Scanning reversed at E = − 1.0 V (black curve), E = − 1.6 V (red curve), E = − 1.8 V (blue curve), E = − 2.0 V (green curve).

Spectroscopic Data

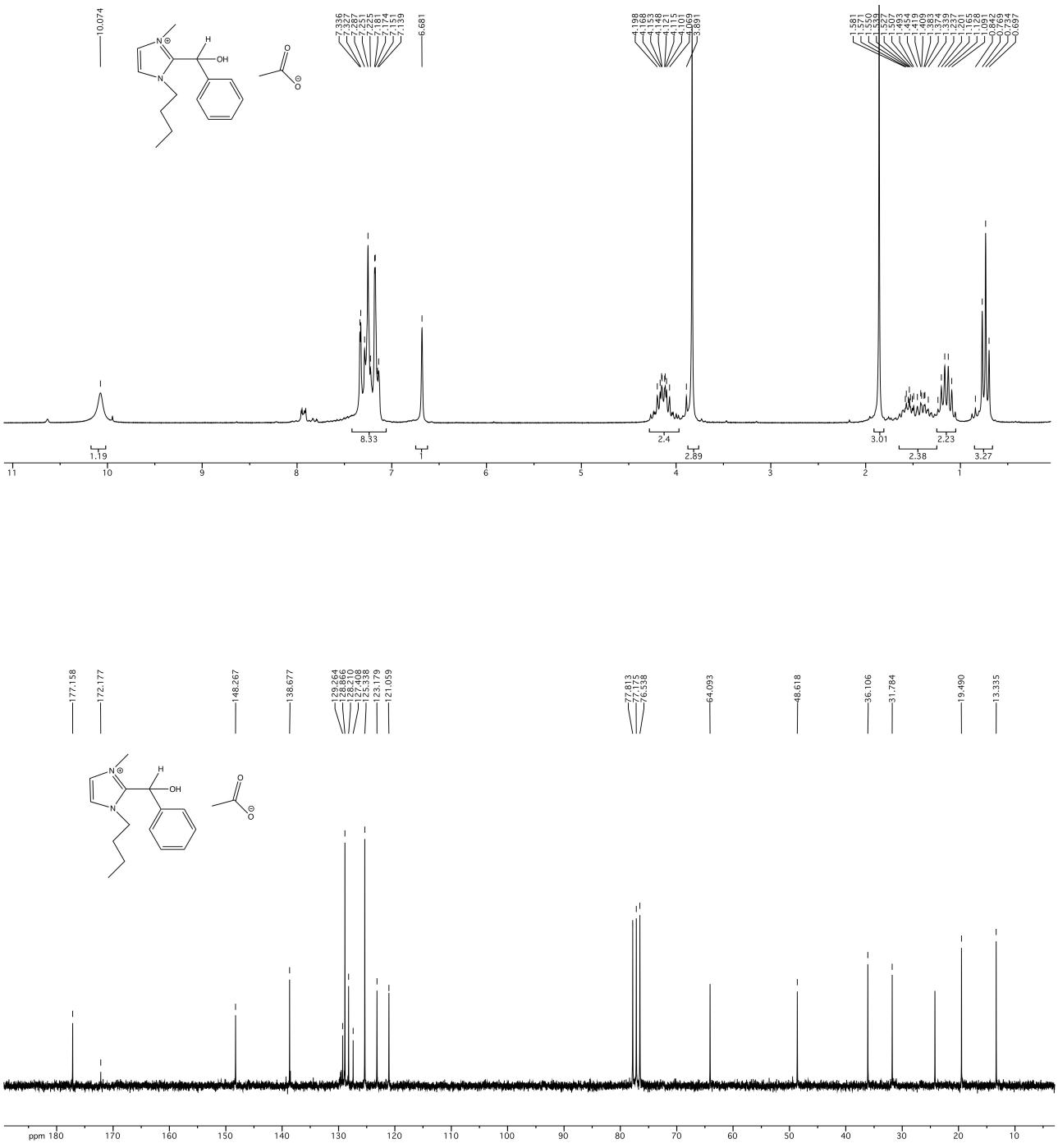

Figure S3 ^{1}H and ^{13}C NMR spectra of (1-butyl-3-methylimidazol-3-ium-2-yl)-phenylmethanol acetate

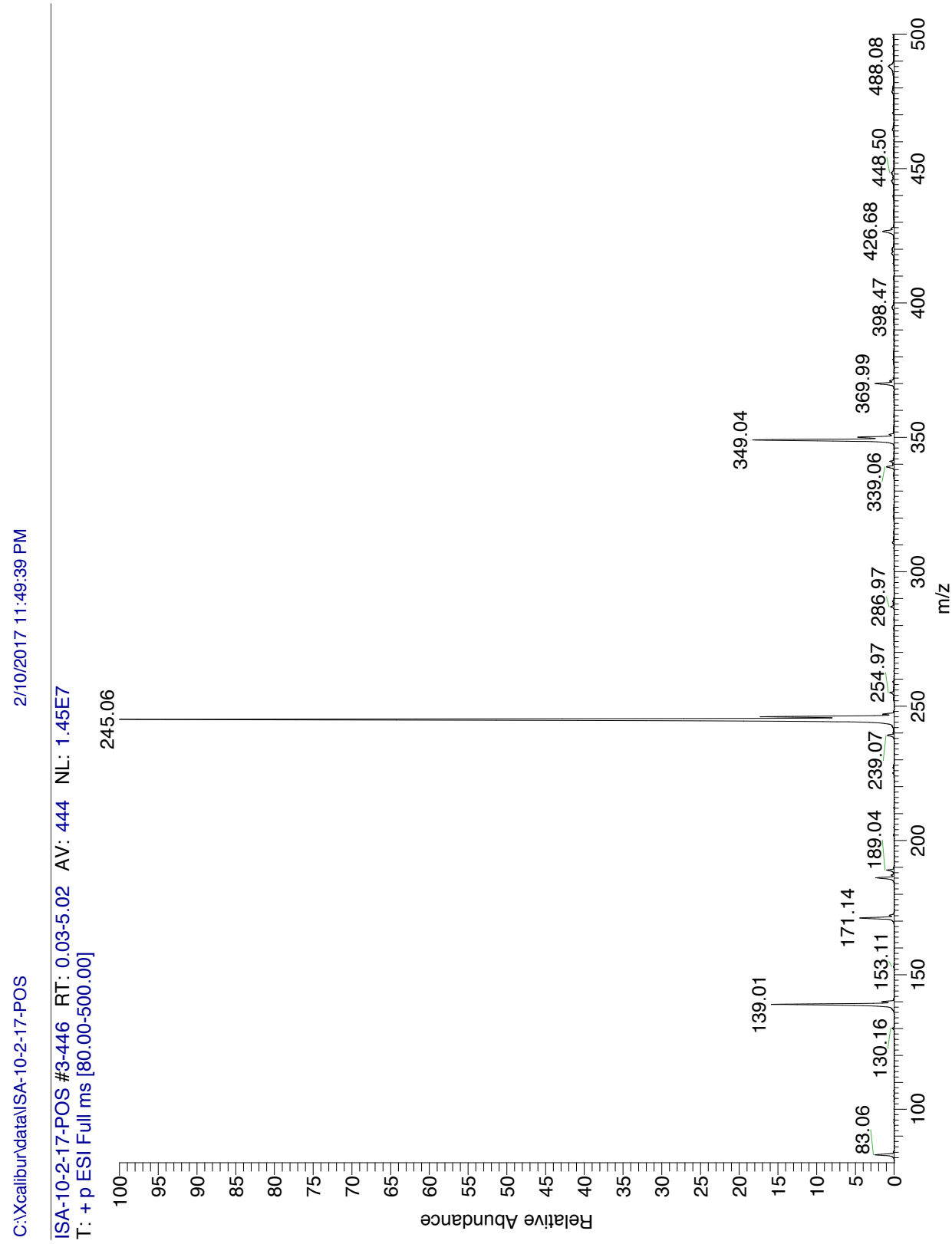

Figure S4 Positive ion ESI mass spectrum of reaction mixture containing BMImAcO and adduct with benzaldehyde.