NMR: A POWERFUL TOOL TO CHARACTERIZE PROTIC IONIC LIQUIDS

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INTRODUCTION

Protic ionic liquids (PILs) are potential candidates to replace organic solvents[1]. However, the features governing PILs' properties are still unclear. In this framework, NMR becomes a powerful tool to provide structural information and describe the dynamical behavior of PILs.

EXPERIMENTAL

- 1D ^{1}H NMR → ΔpKa
- 1D ^{15}N NMR → protonation of the base
- PFG-NMR → charge transport

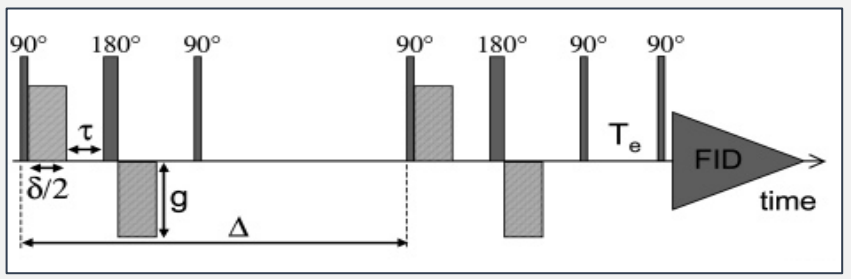
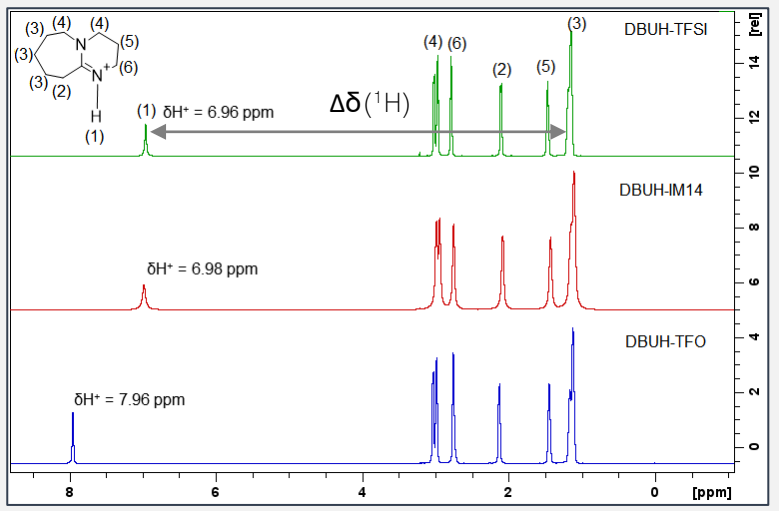


Fig. 1. Schematic view of the BPP LED PFG sequence used in this work[2]

RESULTS



DBUH-TFSI
Δδ(^{1}H) = 5.8 ppm
ΔpKa = 23.4

DBUH-IM14
Δδ(^{1}H) = 5.8 ppm
ΔpKa ≈ 23.4

DBUH-TFO
Δδ(^{1}H) = 6.8 ppm
ΔpKa = 20.4

Fig. 2. 1D ^{1}H NMR spectra of the PILs studied

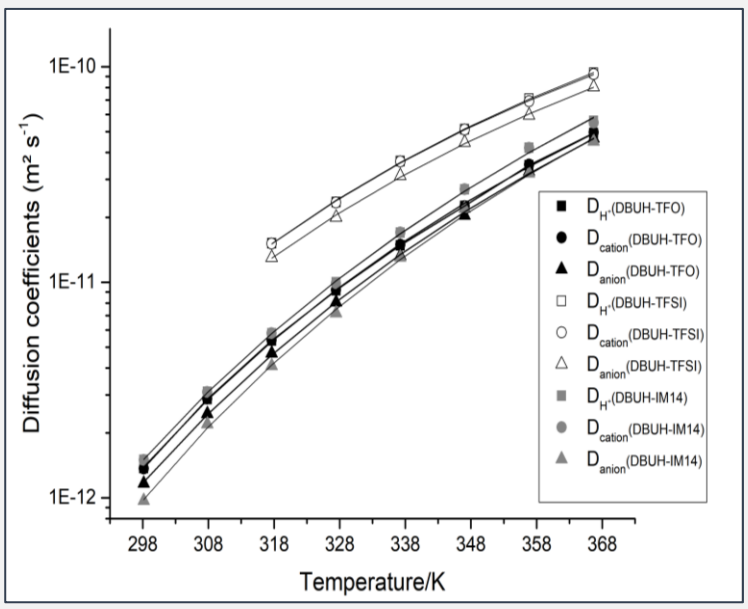


Fig. 4. Self-diffusion coefficients of the ionic species

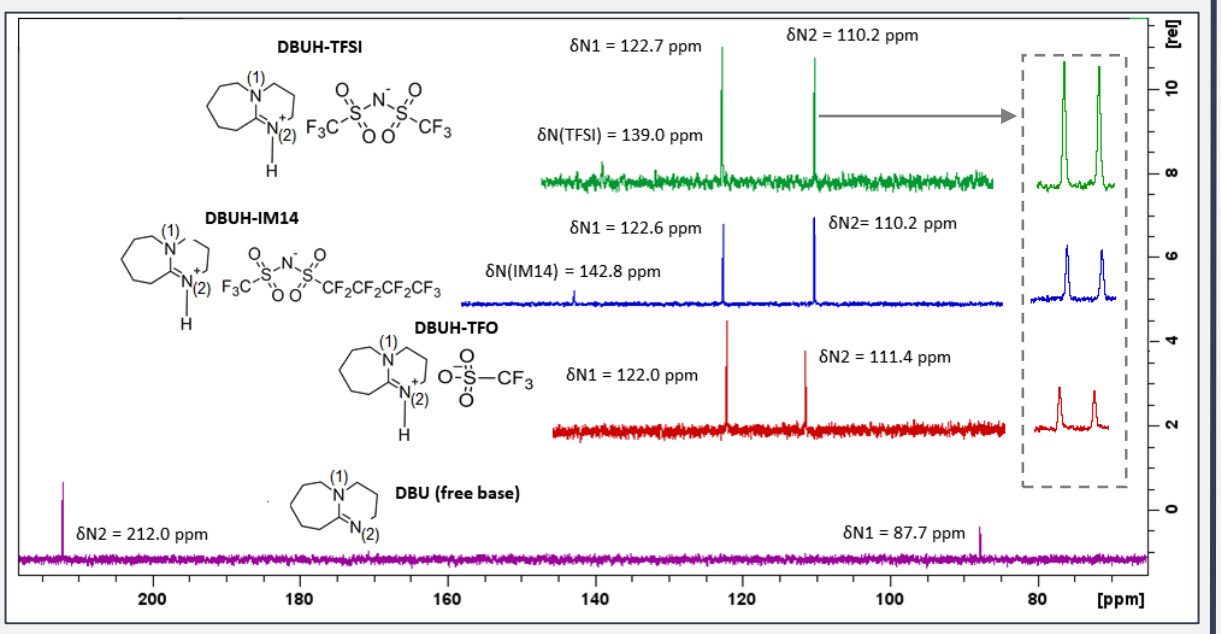


Fig. 3. 1D ^{15}N-{^{1}H} NMR spectra of PILs studied. In the dashed square are the signals of the N2 recorded without ^{1}H decoupling. In all PILs $^{1}J_{N\text{-}H}$ ≈ 97 Hz.

CONCLUSIONS

NMR provides structural and dynamic information about PILs. In the present work, ^{15}N NMR showed the site of protonation of the DBU base. Also, ^{15}N coupled spectra revealed a stable N-H bonding between the H^+ and the imino nitrogen. PFG-NMR results showed the acidic proton moving with the protonated base as a vehicular mechanism of charge transport.

References: [1] Macfarlane et al., 2014, Energy and Environ. Sci., 7, 232–250 [2] A. N. Galatanu et al., 2005," *J. Phys. Chem. B*, 109, 11332–11339.