

Electronic Supplementary Information

Structure, hydrogen bond dynamics and phase transition in a model ionic liquid electrolyte.

Alexander E. Khudozhitkov^{a,d}, Peter Stange^b, Alexander G. Stepanov^a, Daniil I. Kolokolov^{a,d*}, Ralf Ludwig^{b,c,*}

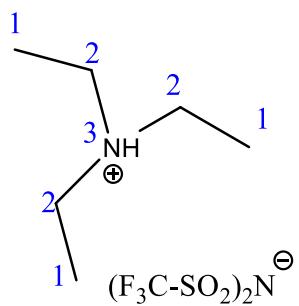
a Boreskov Institute of Catalysis, Siberian Branch of Russian Academy of Sciences, Prospekt Akademika Lavrentieva 5, Novosibirsk 630090, Russia; E-mail: kdi@catalysis.ru

b Universität Rostock, Institut für Chemie, Abteilung für Physikalische Chemie, Dr.-Lorenz-Weg 2, 18059 Rostock, Germany; Tel: 49 381 498 6517; E-mail: ralf.ludwig@uni-rostock.de

c Leibniz-Institut für Katalyse an der Universität Rostock e.V., Albert-Einstein-Str. 29a, 18059 Rostock (Germany)

d Novosibirsk State University, Pirogova Street 2, Novosibirsk 630090, Russia

NMR of [TEA][NTf₂]



| N° | δ (ppm) | Signal | Integration |
|----|----------------|--------|-------------|
| 3 | 8.84 | S | 1 |
| 2 | 3.10 | Q | 6 |
| 1 | 1.17 | T | 9 |

Solid state NMR spectra of [TEA][NTf₂], [TEA][OTf] and [TEA][OMs]

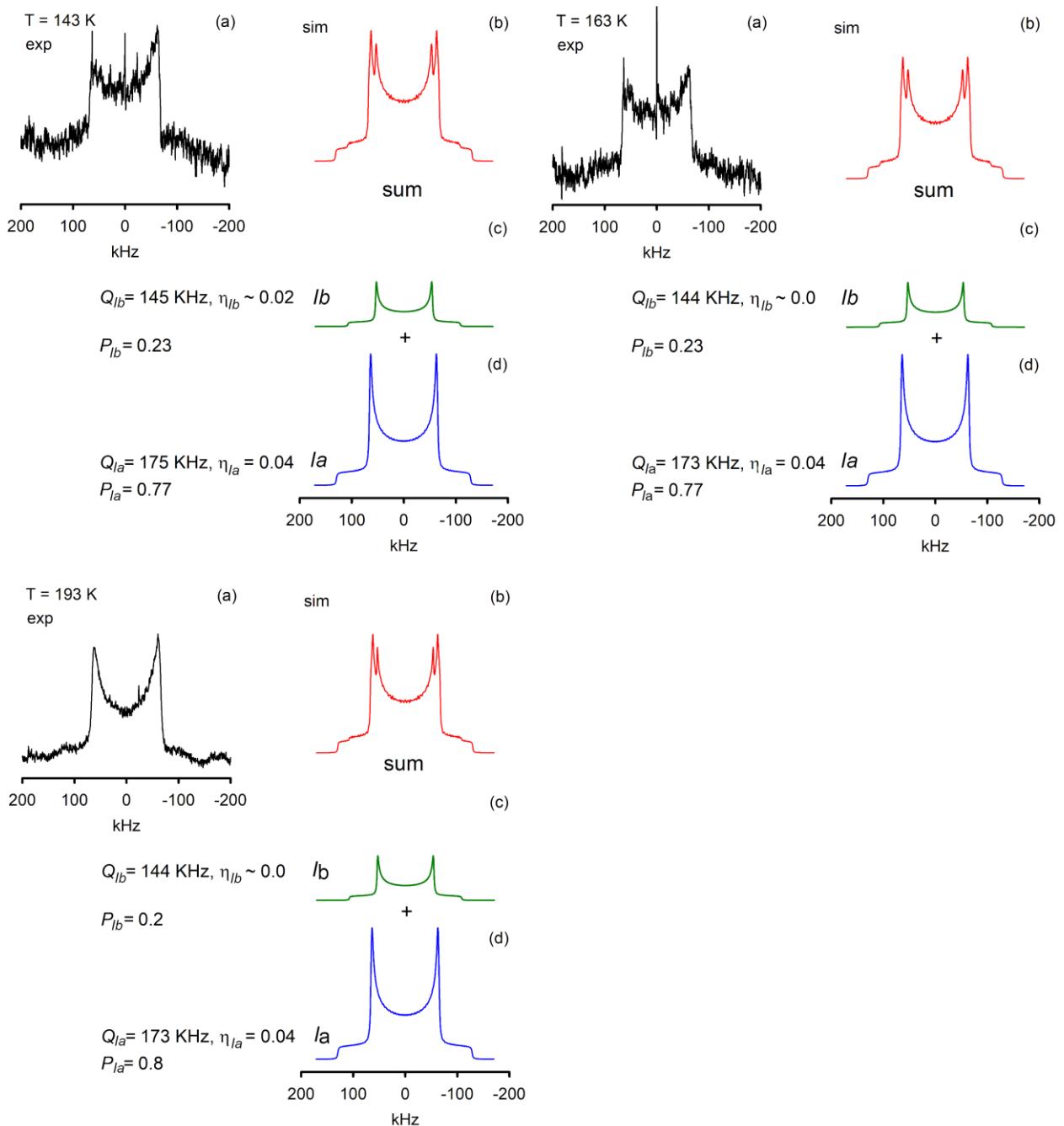


Figure S1. ^2H NMR spectra of [TEA][NTf₂] at 143 K, 163 K and 193 K: For each temperature we show the (a) experimental, (b) simulated and (c-d) the deconvoluted spectra.

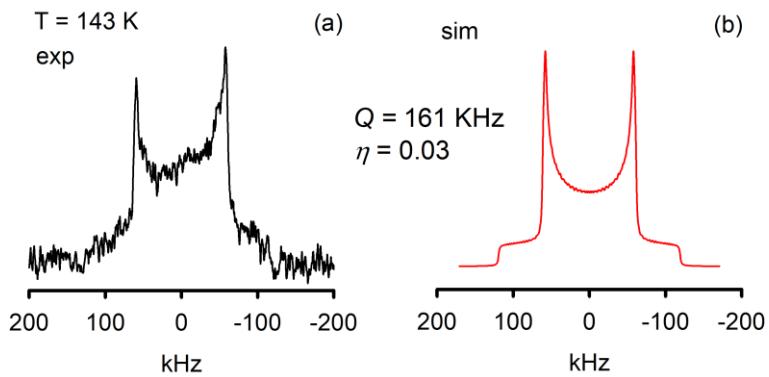


Figure S2. ^2H NMR spectra of [TEA][OTf] at 143 K: (a) experimental, (b) simulated spectra.

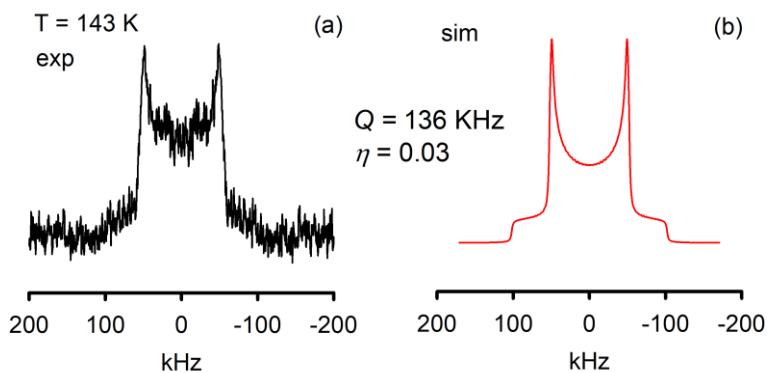


Figure S3. ^2H NMR spectra of [TEA][OMs] at 143 K: (a) experimental, (b) simulated spectra.

DSC profiles of [TEA][NTf₂], [TEA][OTf] and [TEA][OMs]

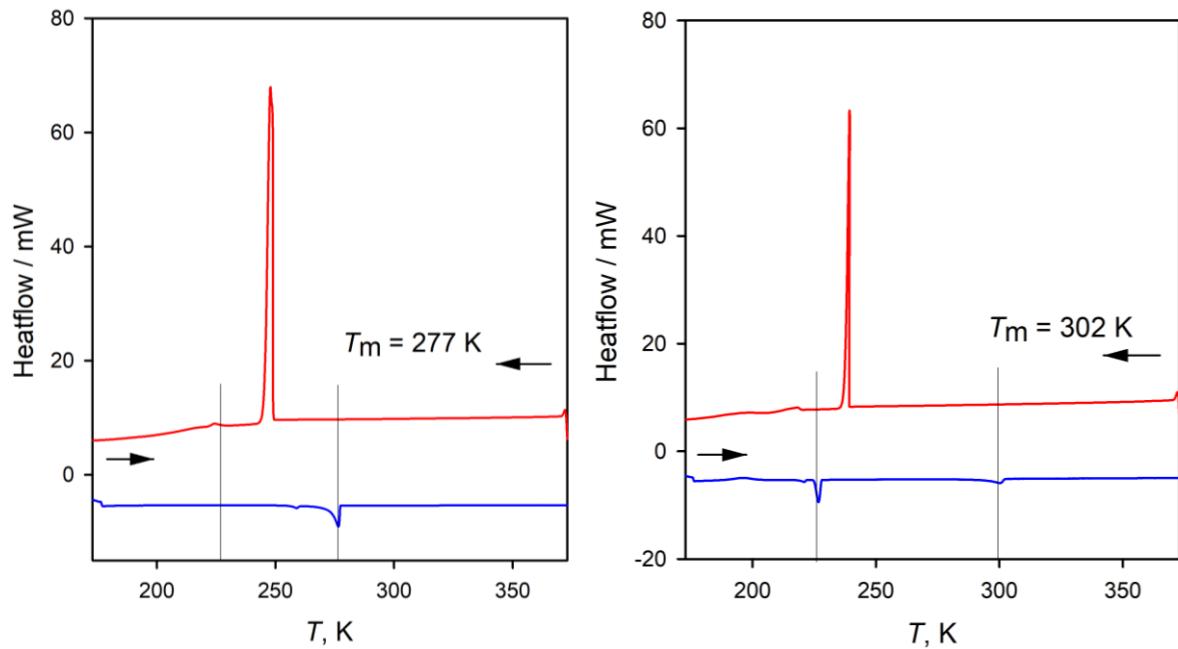


Figure S4 The DSC profile for [TEA][NTf₂] (left) and [TEA][OTf] samples: the heating rate was $1 \text{ K} \cdot \text{min}^{-1}$.

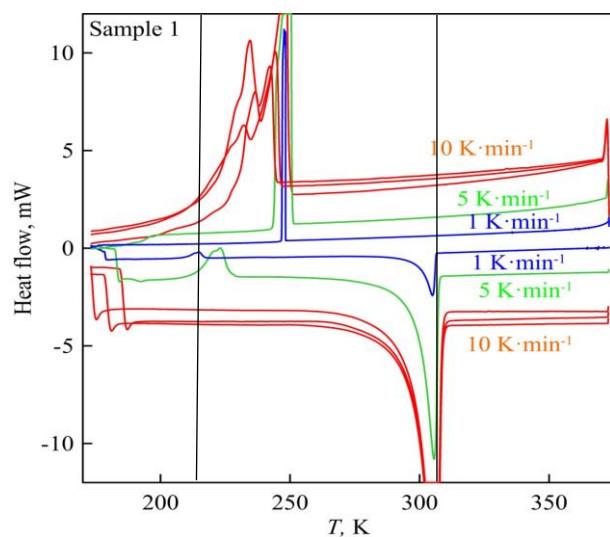


Figure S5. The DSC profile for [TEA][OMs] samples; blue line is cooling and heating with $1 \text{ K} \cdot \text{min}^{-1}$, green lines corresponds to cooling and heating with $5 \text{ K} \cdot \text{min}^{-1}$, red line - $10 \text{ K} \cdot \text{min}^{-1}$. The curves with the same heating or cooling rate are shifted for 0.1 mW for better illustration.