96 hour aerobic thermolysis of PPN$^+$X$^-$ salts at 200 °C, 250 °C, and 300 °C. An evaluation of anion suitability for use in ionic liquids with long-term, high-temperature thermal stability

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SUPPORTING INFORMATION

- DSC Traces for all salts (1-14)
- Electrostatic potential maps for the Sac$^-$ and BDSA$^-$ anions, and computational details
- Multinuclear NMR spectra of all new salts (5, 6, 8, 10, 11, 14)
Differential Scanning Calorimetry
Top to Bottom: 1, 2, 3, 4, 5.
Differential Scanning Calorimetry
Top to Bottom: 6, 7, 8.
Differential Scanning Calorimetry
Top to Bottom: 9, 10, 11, 12.
Differential Scanning Calorimetry

Top to Bottom: 13, 14.
Electrostatic potential energy surface plots for Sac´ (left) and BDSA´ (right) generated by Spartan'08
[computational model: B3LYP/6-311+G(d,p)].

Color range: -551(red) to -102 (blue) kJ/mol. Selected local extrema are indicated. For Sac´, the most
negative site is associated with the carbonyl oxygen at -551 kJ/mol, followed closely by a site near the
imidate N at -549 kJ/mol; the regions about the sulfonyl O atoms (orange) are generally not as negative
as the imidate N or the carbonyl oxygen (red). The imidate moiety of BDSA´ is comparatively less
negative than its counterpart in Sac´; the most negative site on Sac´ is near the imidate N at -514 kJ/mol.

A-FREHEAT_2.15.17_DAVIS_PROTON-2.jpg

Filename: A-FREHEAT_2.15.17_DA
Author: DAV Scale
Experiment: single_pulse-sac
Sample_ID: A-FREHEAT_2.15.17_DA
Solvent: CHLOROFORM-D
Sample_name: 27
Creation_time: 15-FEB-2017 17:37:29
Revision_time: 15-FEB-2017 18:33:08
Current_time: 15-FEB-2017 18:33:08
Date_format: 1D COMPLEX
Dim_size: 13127
Dim_title: 1H
Dim_units: [ppm]
Dimensions: 1
Site: ECA 503
Spectrometer: JNM-ECA403
Field_strength: 3.7450910 [T] (500 [MHz])
N_acq_Duration: 1.17 [s]
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K_offset: 6.50 [ppm]
K_points: 2048
K_resolution: 0.06797727 [Hz]
K_sweep: 2.843242 [kHz]
Irre_freq: 6.9 [ppm]
Irre_offset: 500.1599531 [MHz]
Tri_Domain: 1H
Tri_offset: 6.2 [ppm]
Tri_freq: 500.1599531 [MHz]
Clipped: FALSE
Mod_return: 16
Scan: 16
Total_scans: 16
K_95_width: 13.07 [us]
K_acq_time: 1.17450910 [s]
K_angle: 45 [deg]
K_size: 4 [mm]
K_gains: 6.559 [us]
Irre_mode: OFF
Tri_mode: OFF
Invert_polar: TRUE
Initial_wait: 1 [s]
Recover_pulse: 30
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Temp_set: 210 [OC]

X: parts per Million: 1H

PPN SAC

IL # 6