

Electronic Supporting Information

Halogen-free synthesis of symmetrical 1,3-dialkylimidazolium ionic liquids using non-enolisable starting materials

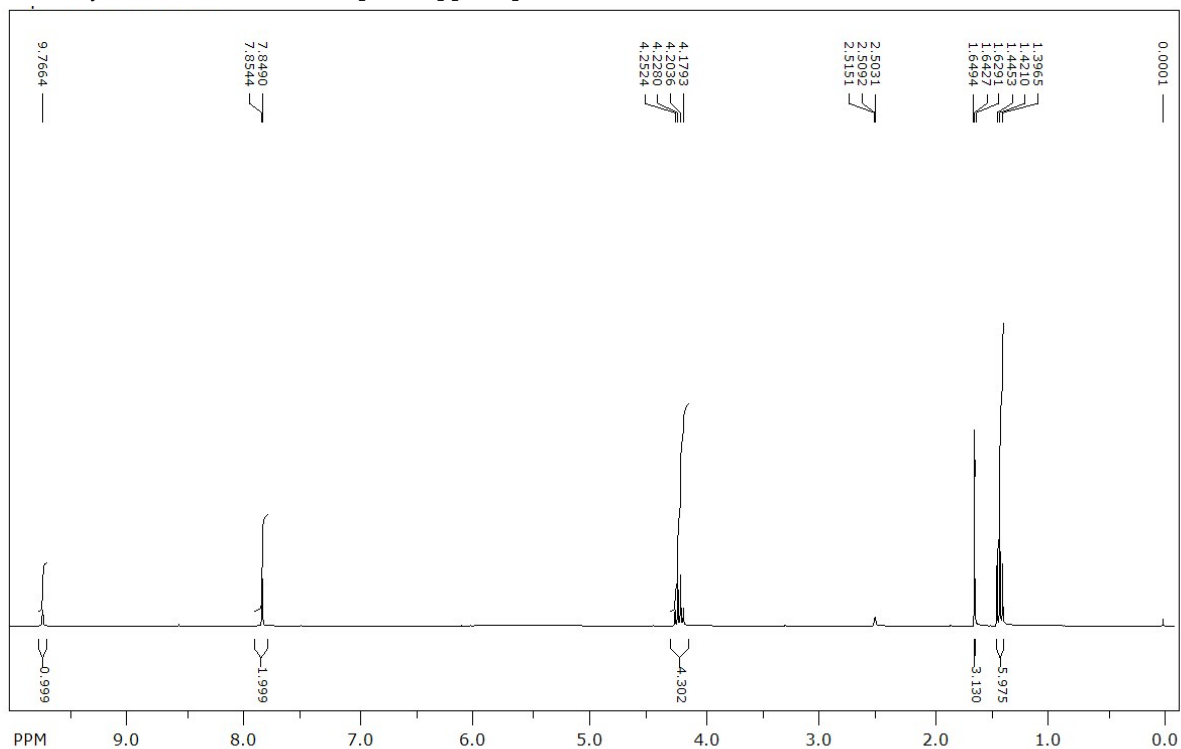
Daphne Depuydt, Arne Van den Bossche, Wim Dehaen, Koen Binnemans*

Experimental

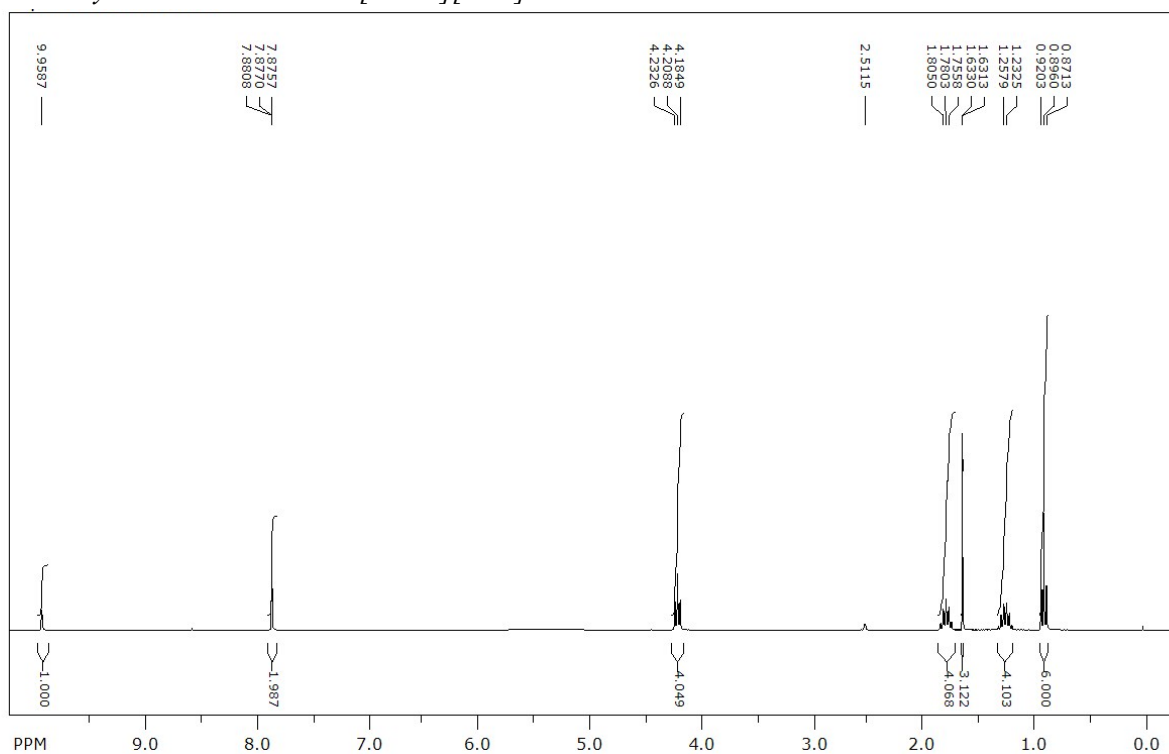
^1H NMR

Acetate ILs

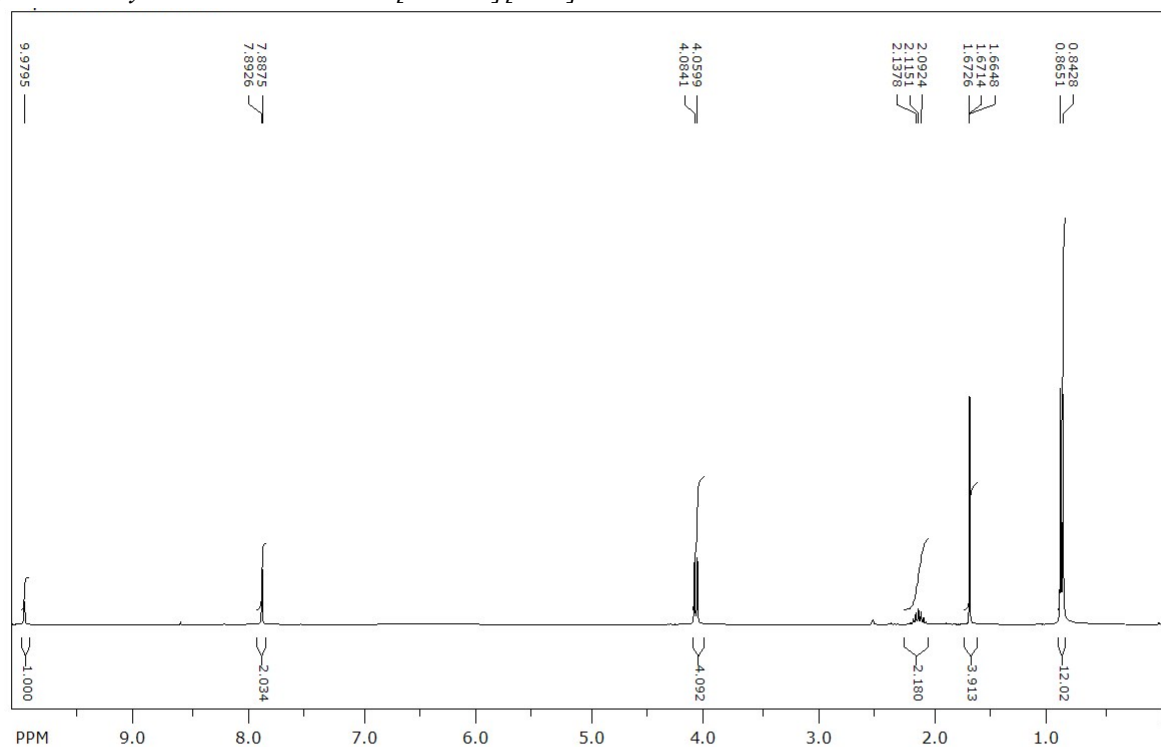
1,3-Diethylimidazolium acetate [EEIM][AcO]



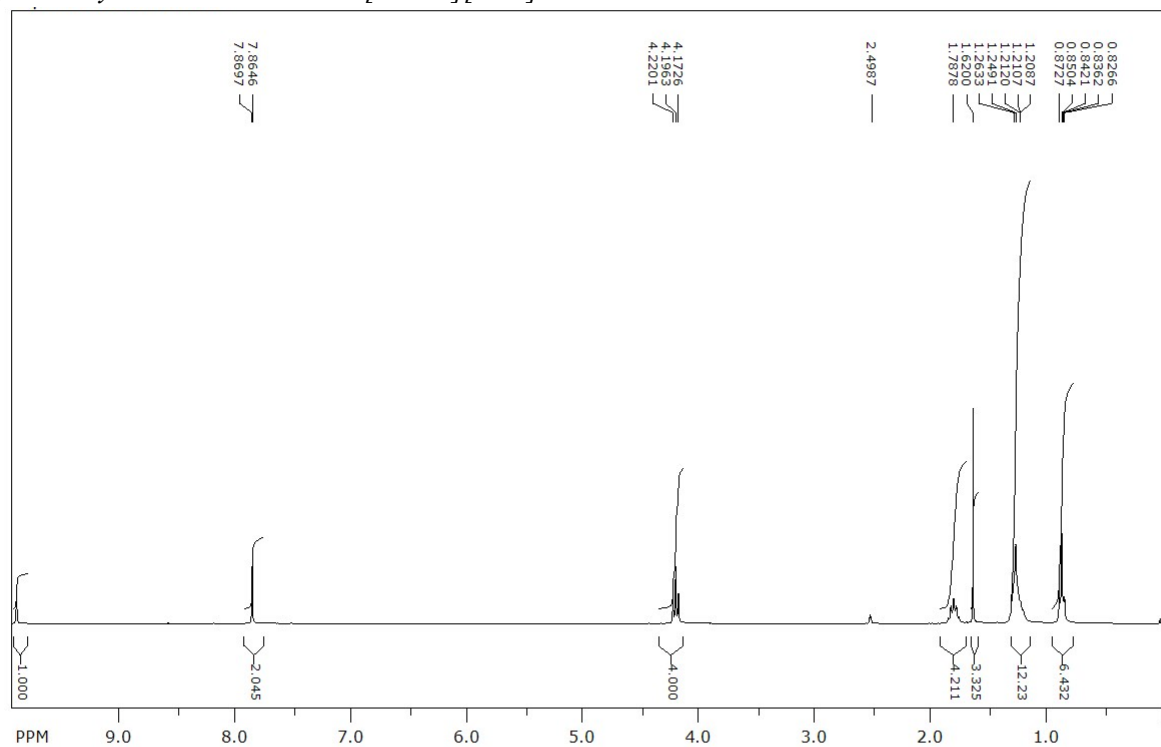
1,3-Dibutylimidazolium acetate [BBIM][AcO]



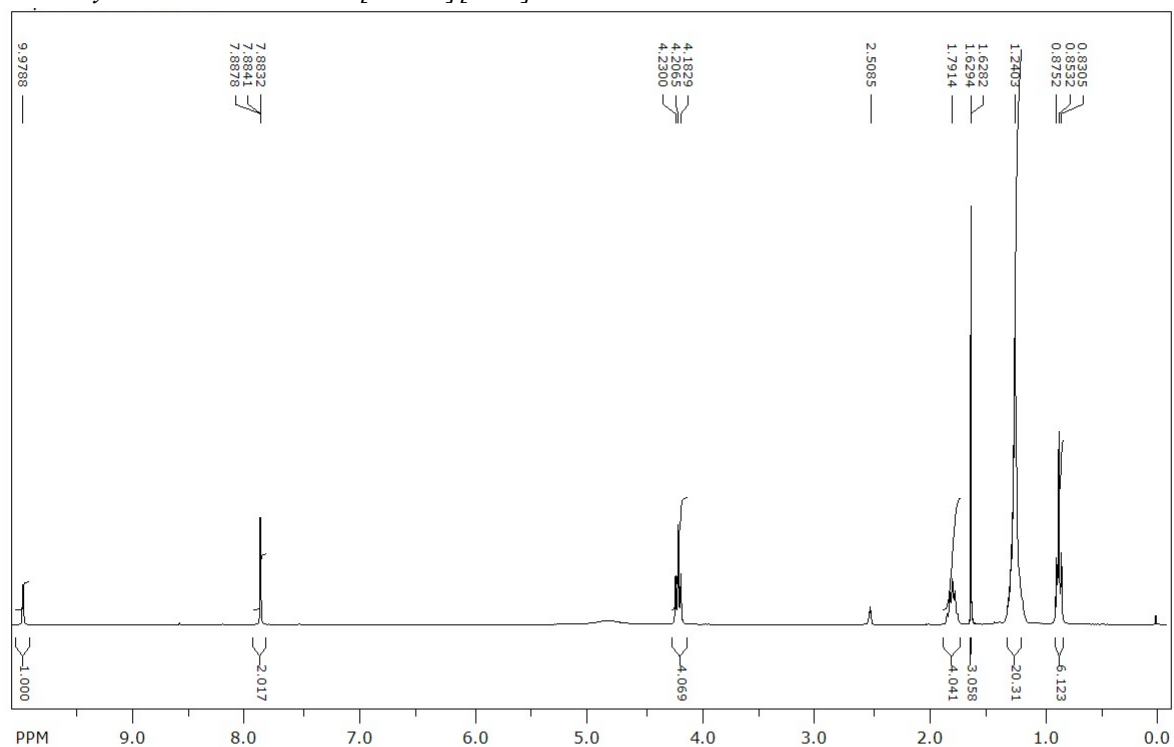
1,3-Diisobutylimidazolium acetate [iBiBIM][AcO]



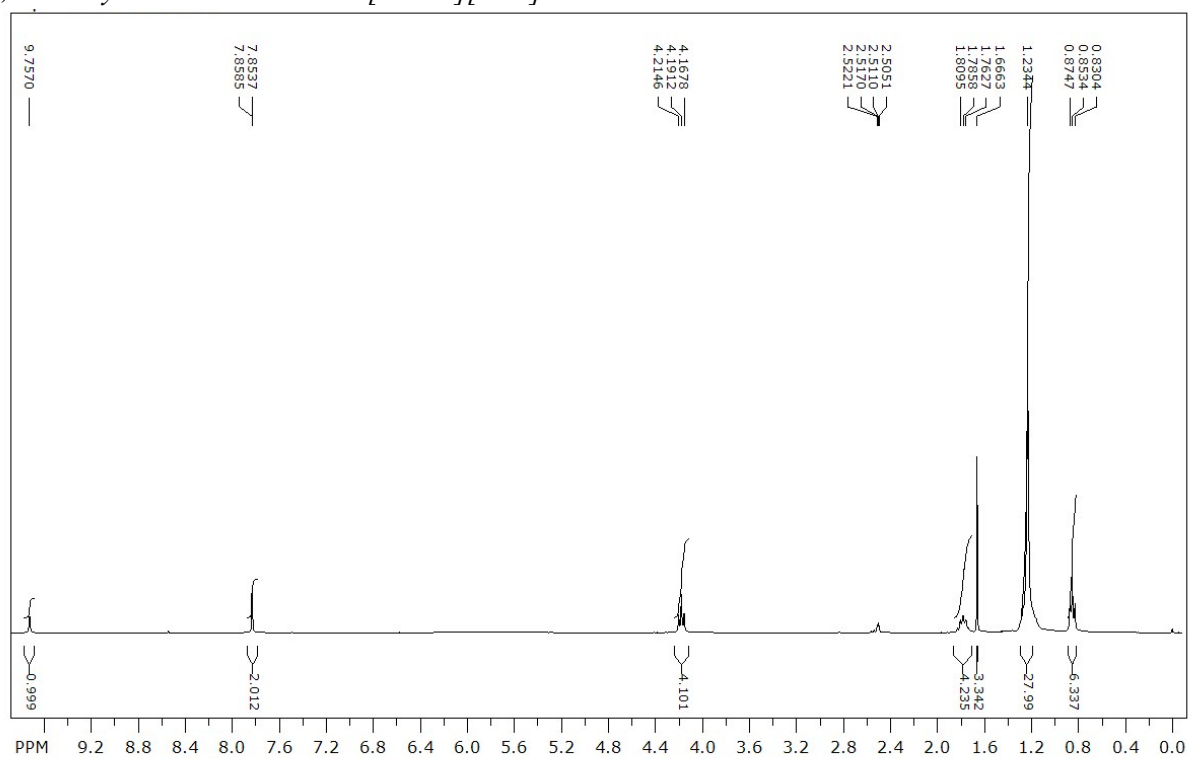
1,3-Dihexylimidazolium acetate [HHIM][AcO]



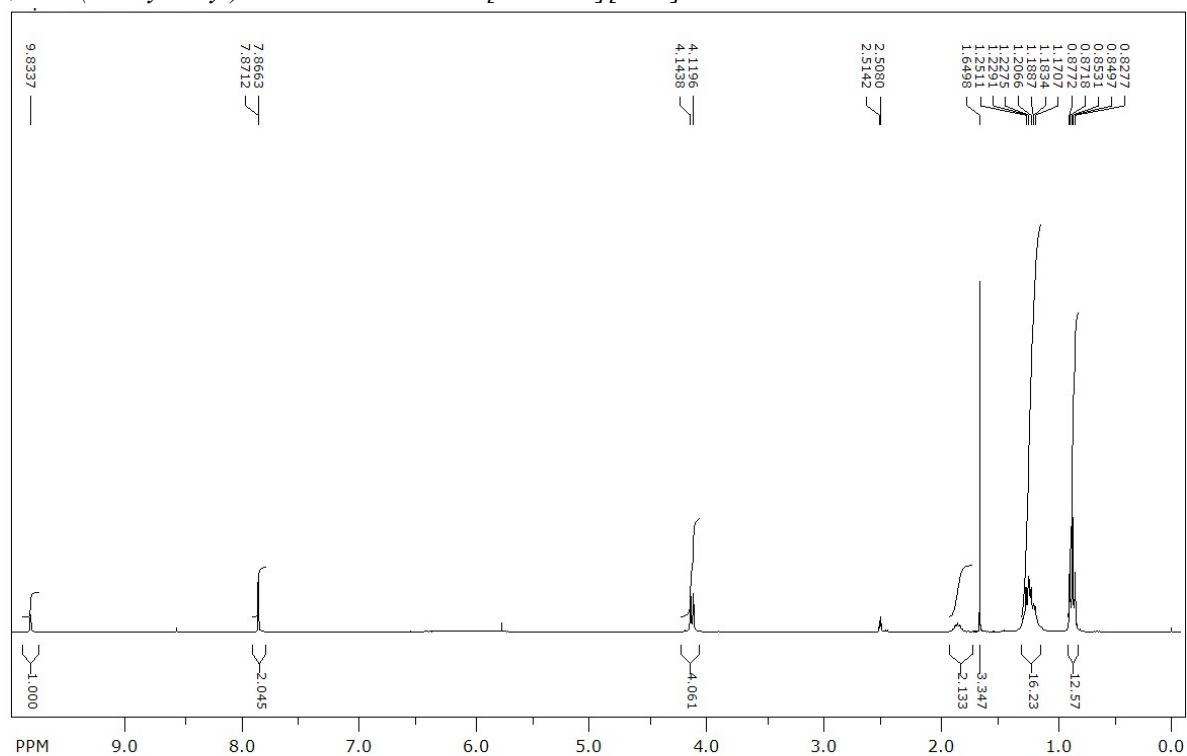
1,3-Dioctylimidazolium acetate [OOIM][AcO]



1,3-Didecylimidazolium acetate [DDIM][AcO]

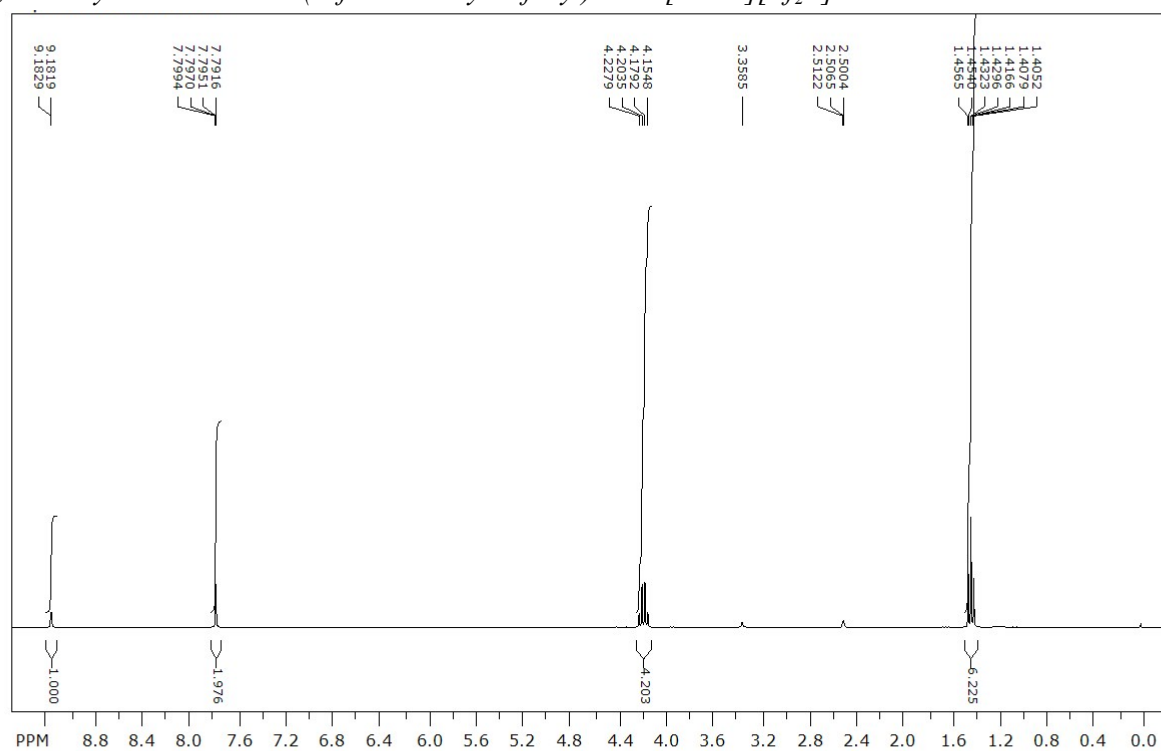


1,3-Bis(2-ethylhexyl)imidazolium acetate [EhEhIM][AcO]

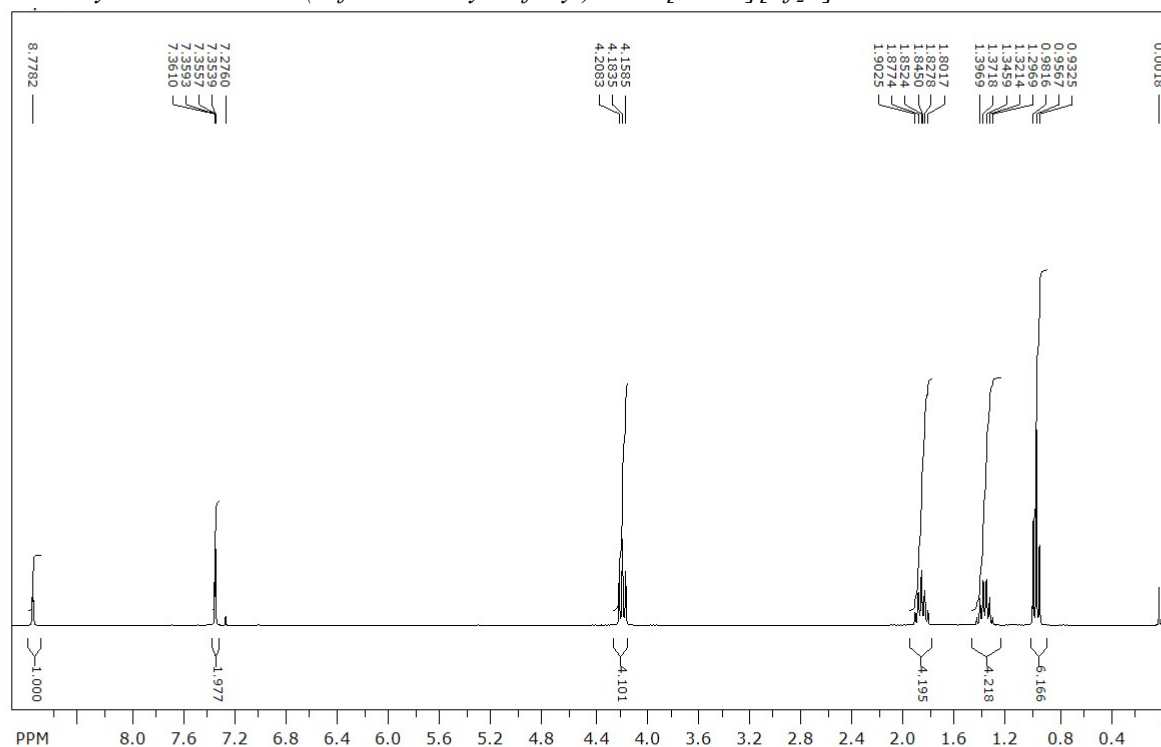


Bis(trifluoromethylsulfonyl)imide ILs

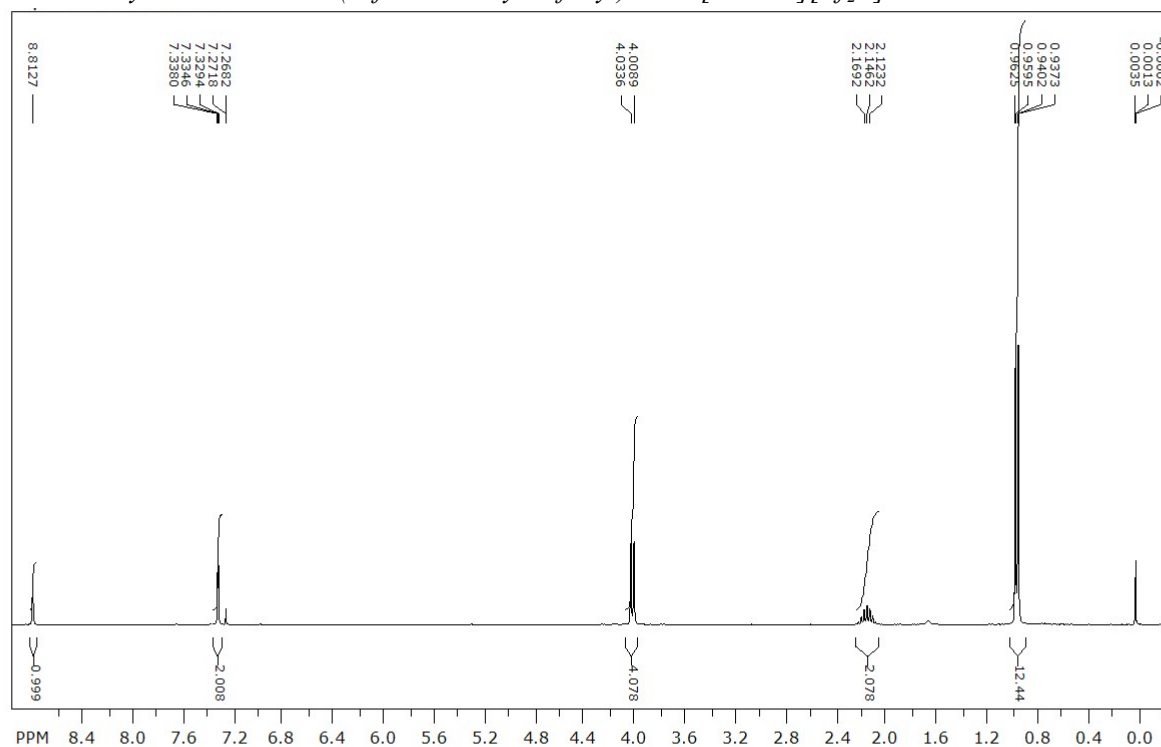
1,3-Diethylimidazolium bis(trifluoromethylsulfonyl)imide [EEIM][Tf₂N]



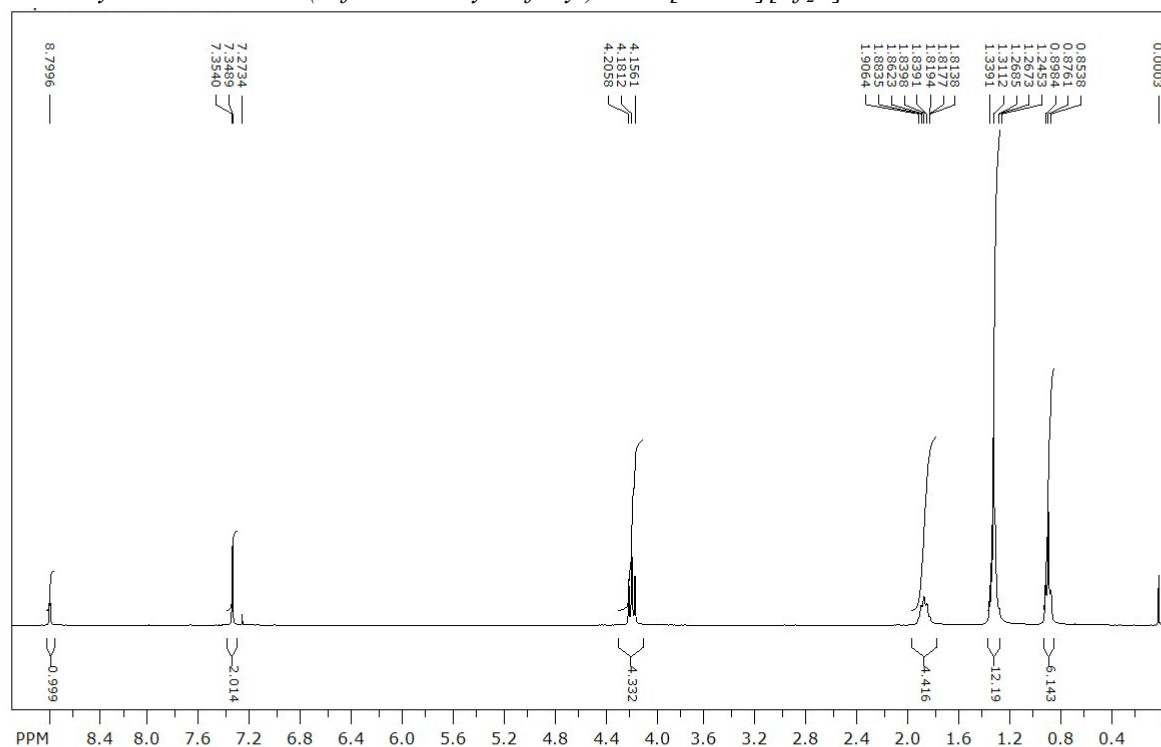
1,3-Dibutylimidazolium bis(trifluoromethylsulfonyl)imide [BBIM][Tf₂N]



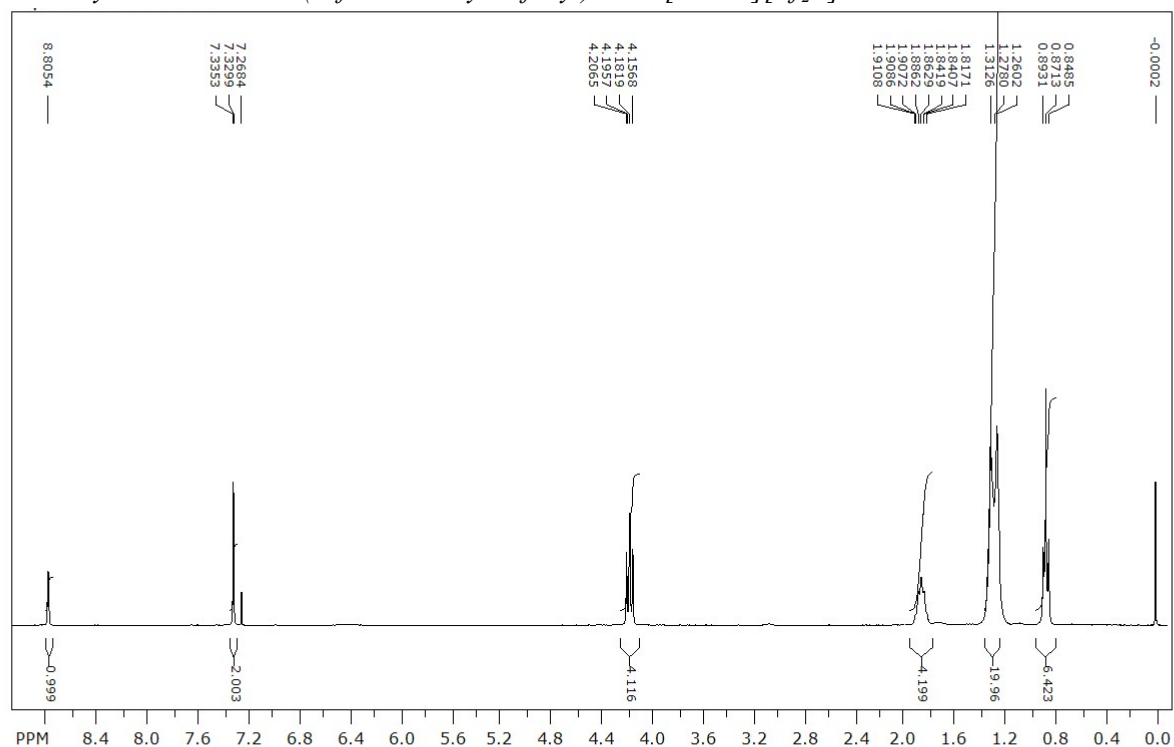
1,3-Diisobutylimidazolium bis(trifluoromethylsulfonyl)imide [iBiBIM][Tf₂N]



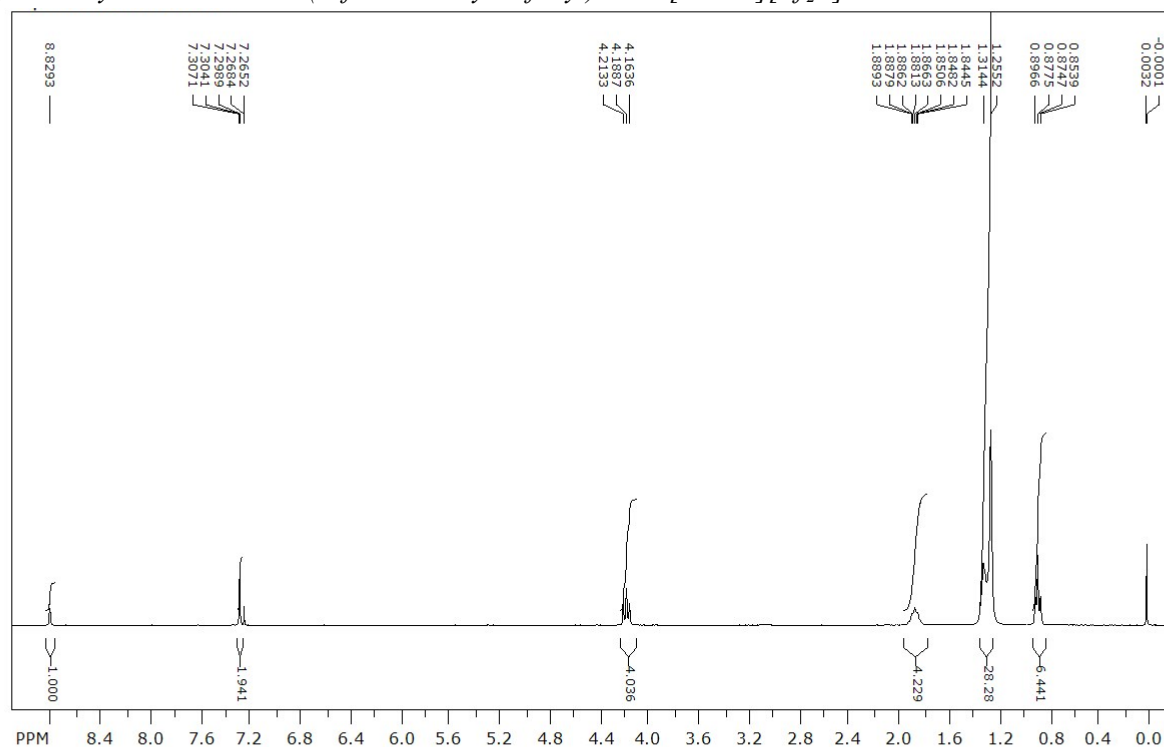
1,3-Dihexylimidazolium bis(trifluoromethylsulfonyl)imide [HHIM][Tf₂N]



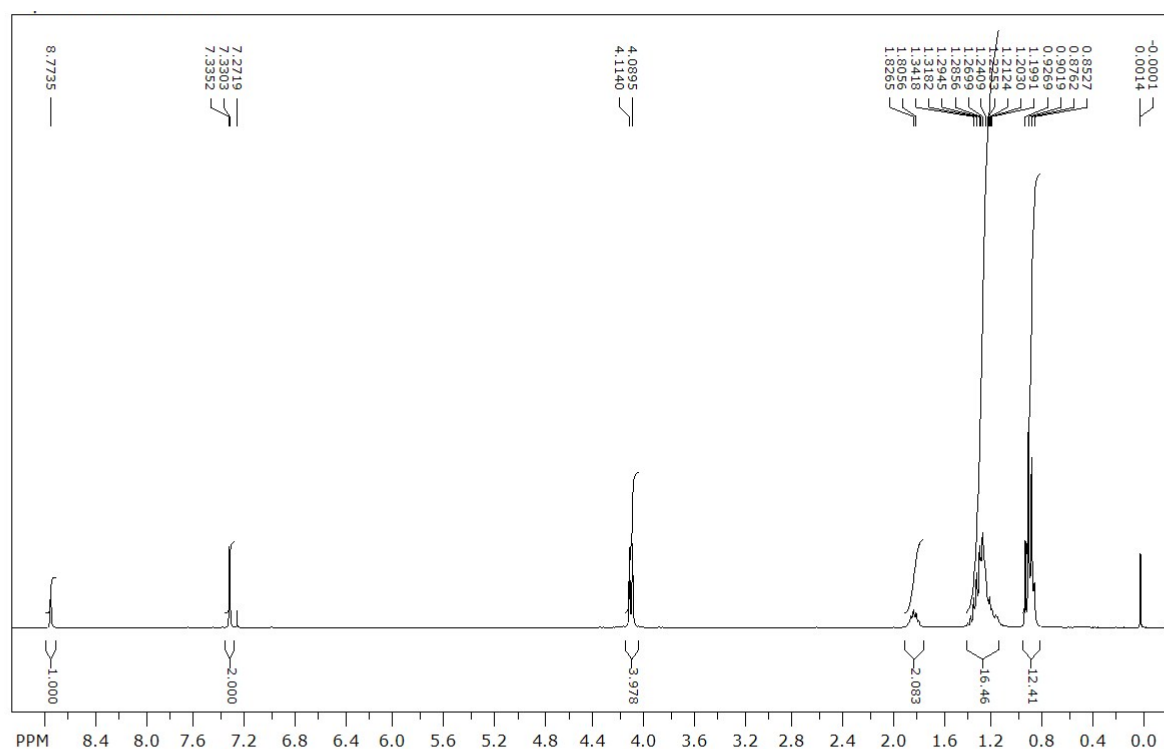
1,3-Dioctylimidazolium bis(trifluoromethylsulfonyl)imide [OOIM][Tf₂N]



1,3-Didecylimidazolium bis(trifluoromethylsulfonyl)imide [DDIM][Tf₂N]

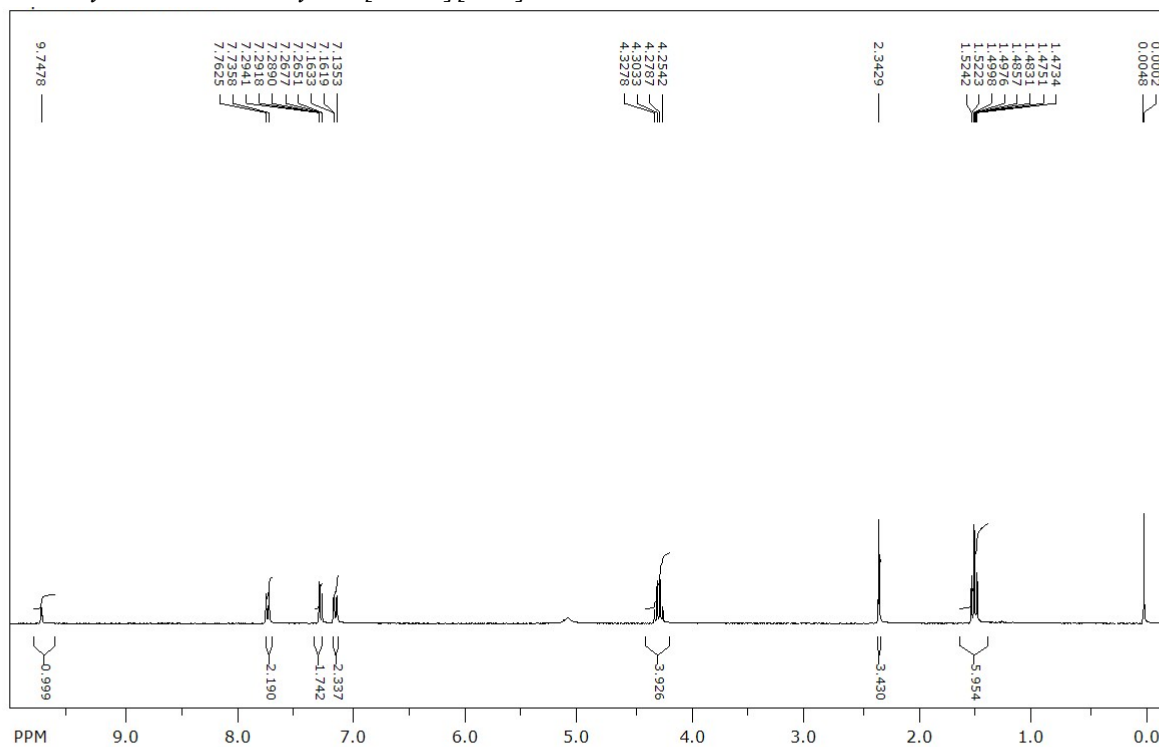


1,3-Bis(2-ethylhexyl)imidazolium bis(trifluoromethylsulfonyl)imide [EhEhIM][Tf₂N]

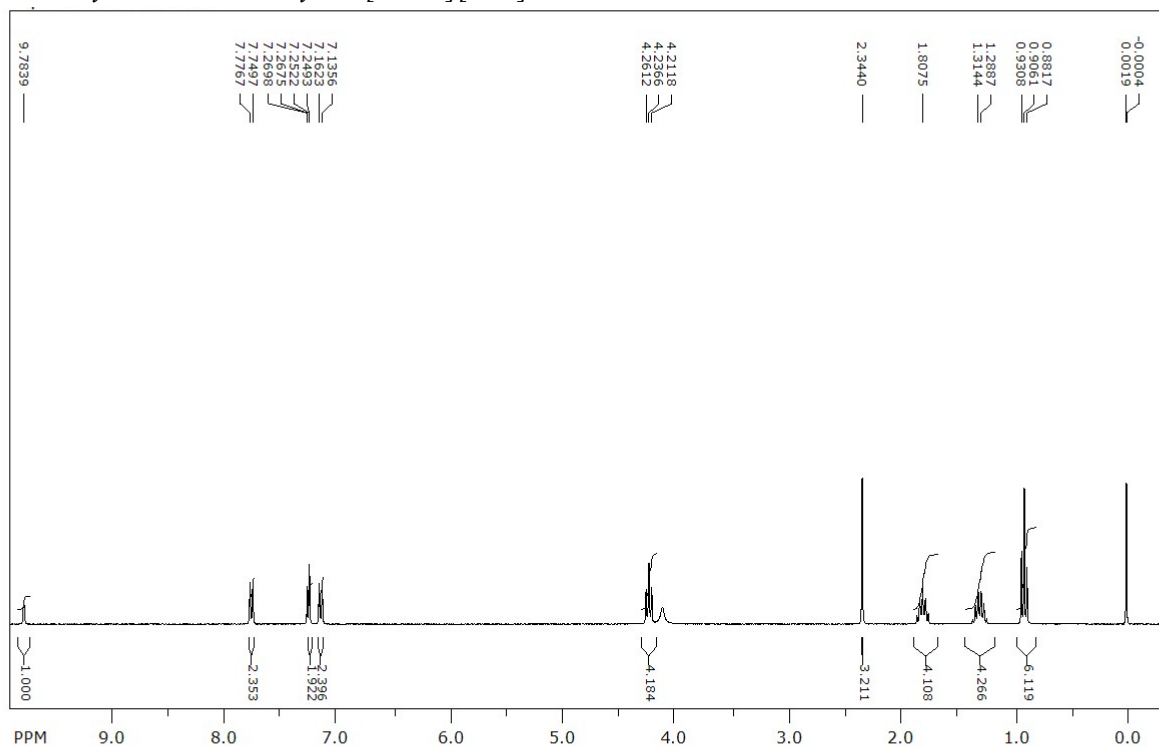


Tosylate ILs

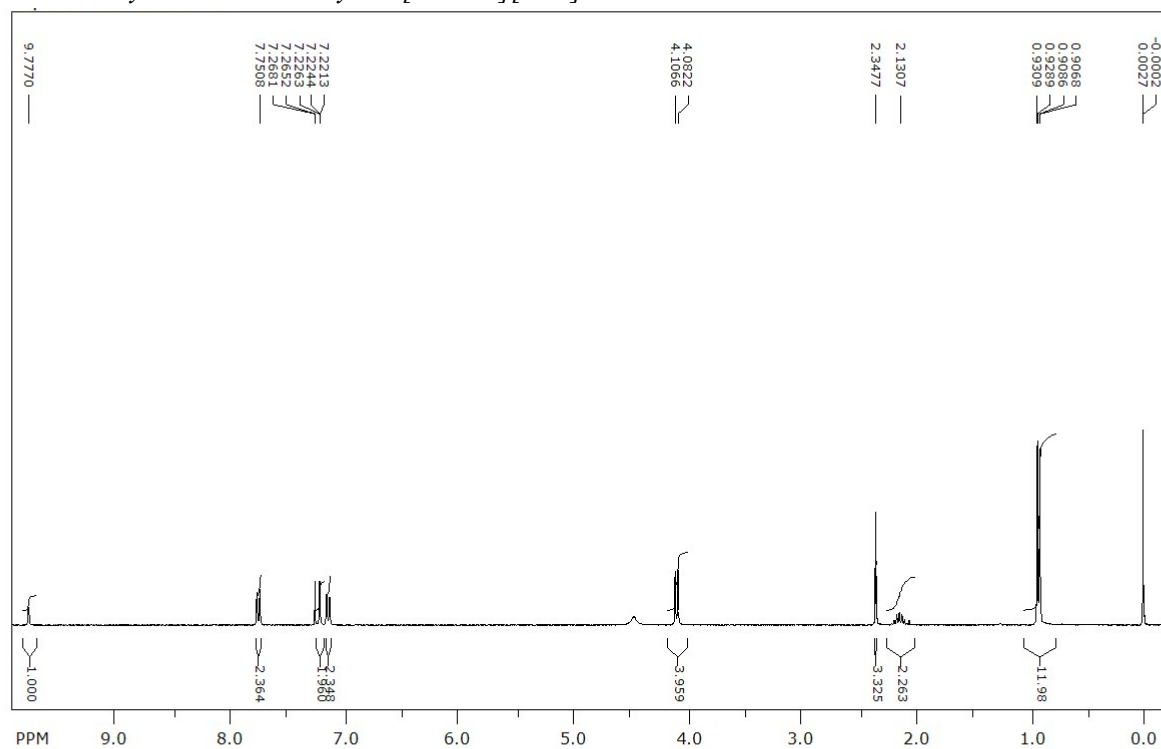
1,3-Diethylimidazolium tosylate [EEIM][OTs]



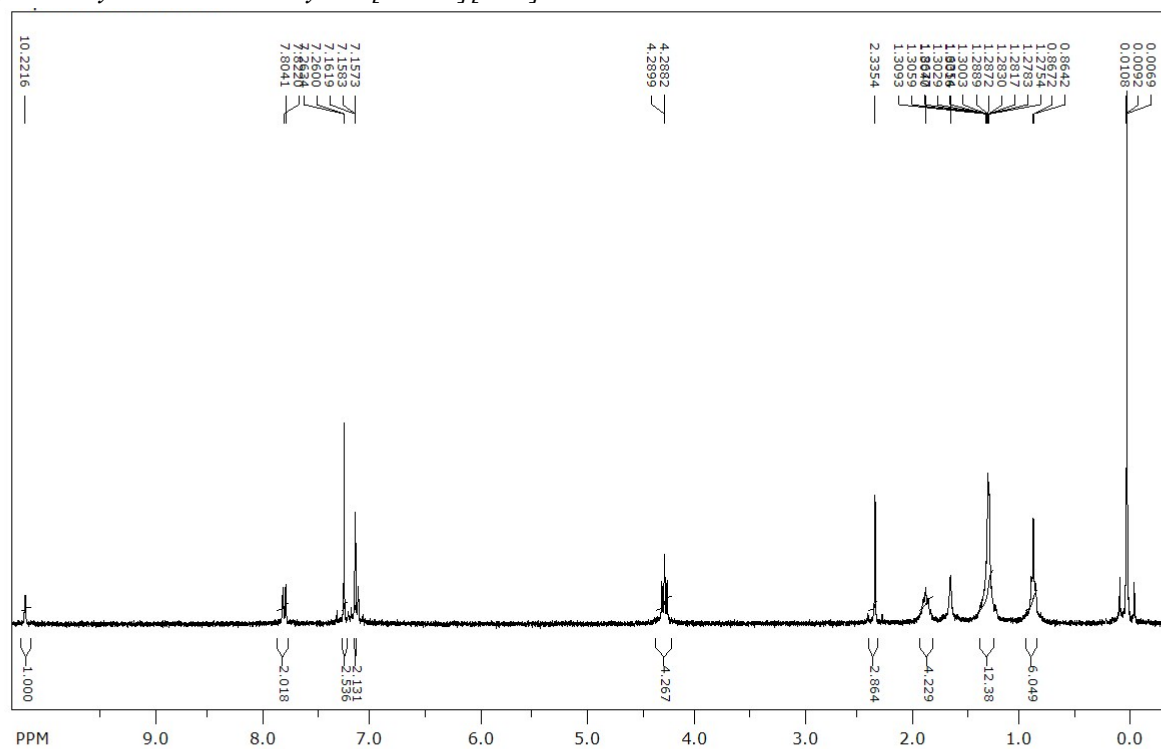
1,3-Dibutylimidazolium tosylate [BBIM][OTs]



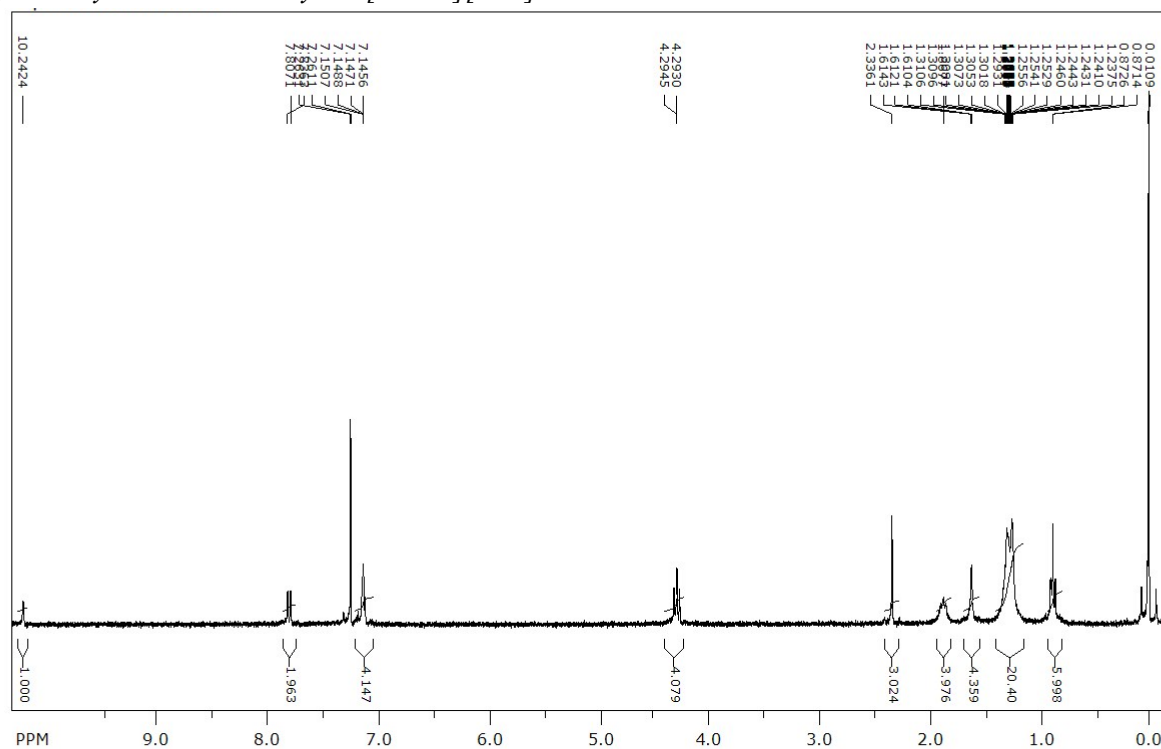
1,3-Diisobutylimidazolium tosylate [iBiBIM][OTs]



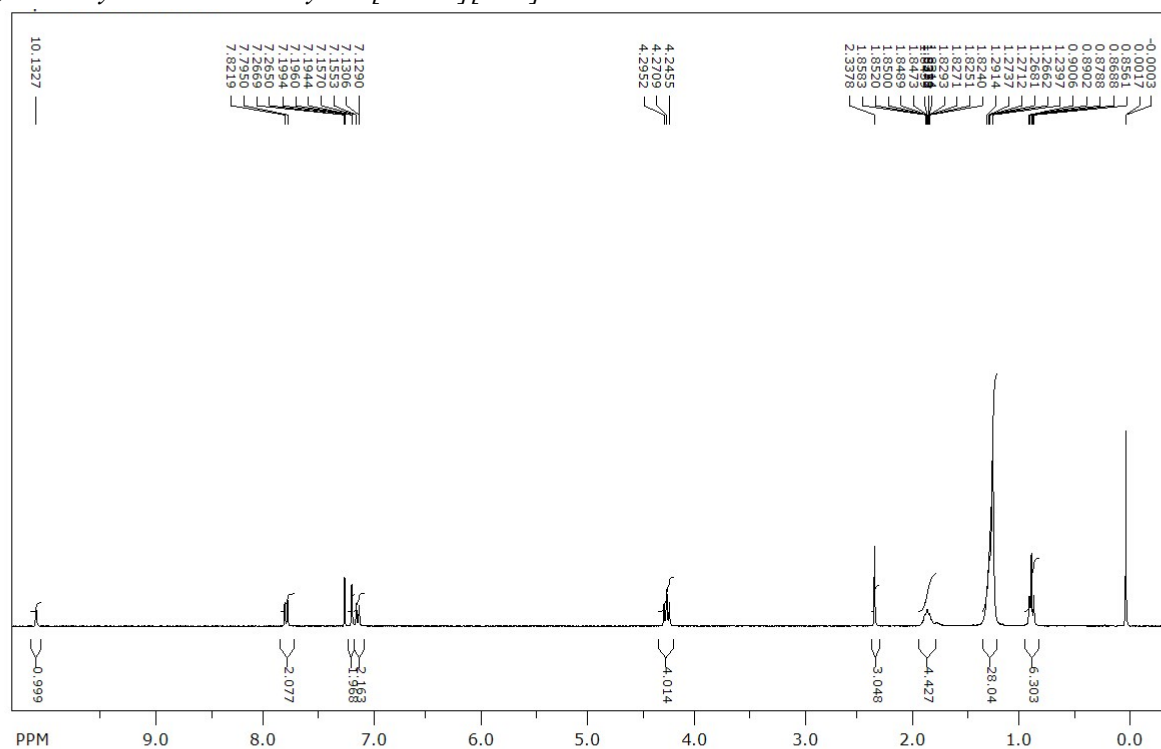
1,3-Dihexylimidazolium tosylate [HHIM][OTs]



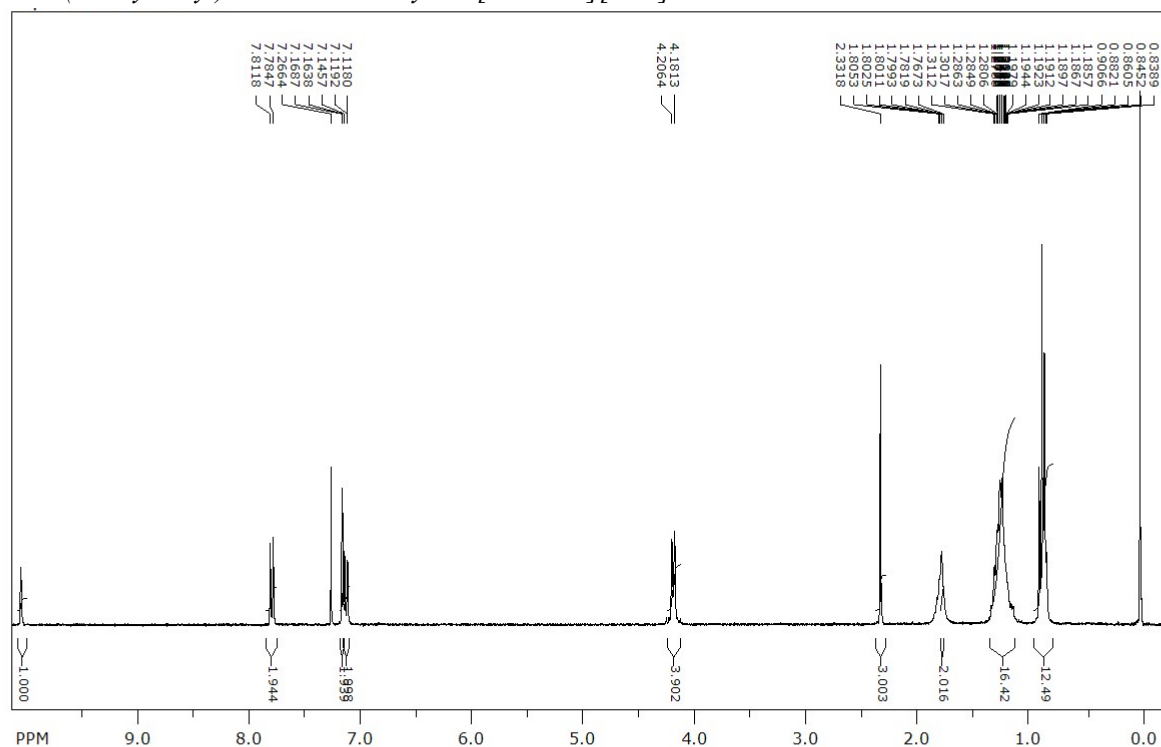
1,3-Dioctylimidazolium tosylate [OOIM][OTs]



1,3-Didecylimidazolium tosylate [DDIM][OTs]

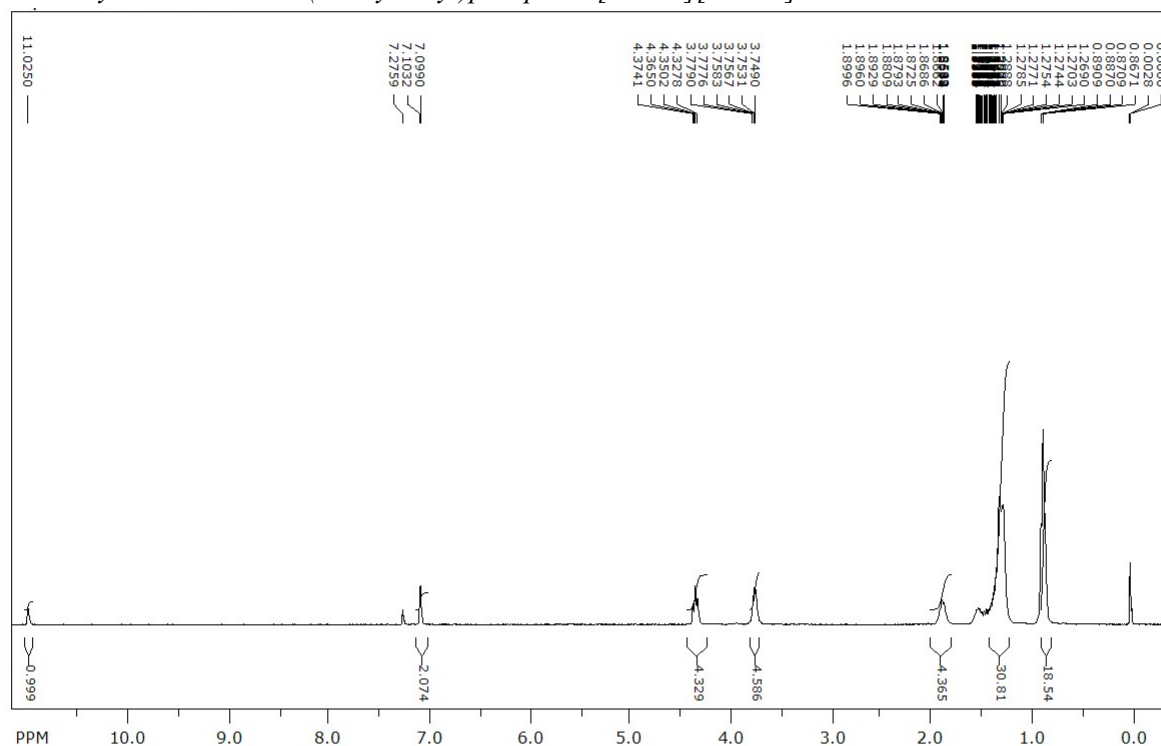


1,3-bis(2-ethylhexyl)imidazolium tosylate [EhEhIM][OTs]

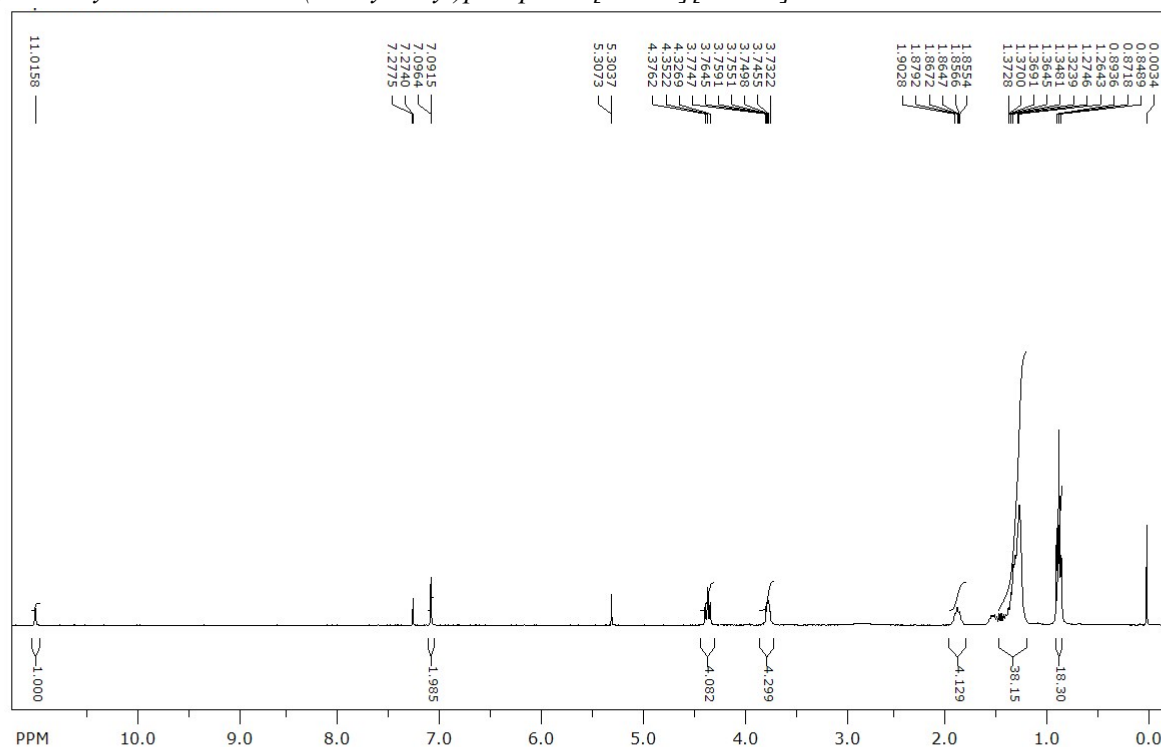


Bis(2-ethylhexyl)phosphate ILs

1,3-Dihexylimidazolium bis(2-ethylhexyl)phosphate [HHIM][DEHP]

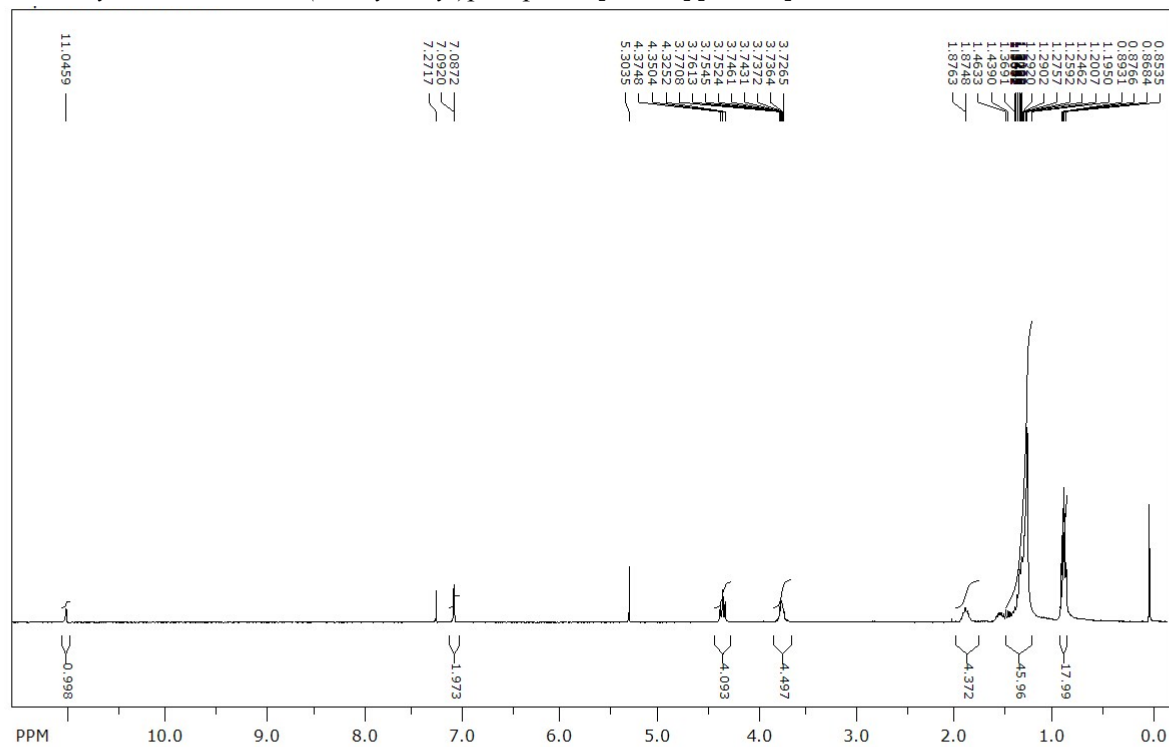


1,3-Dioctylimidazolium bis(2-ethylhexyl)phosphate [OOIM][DEHP]



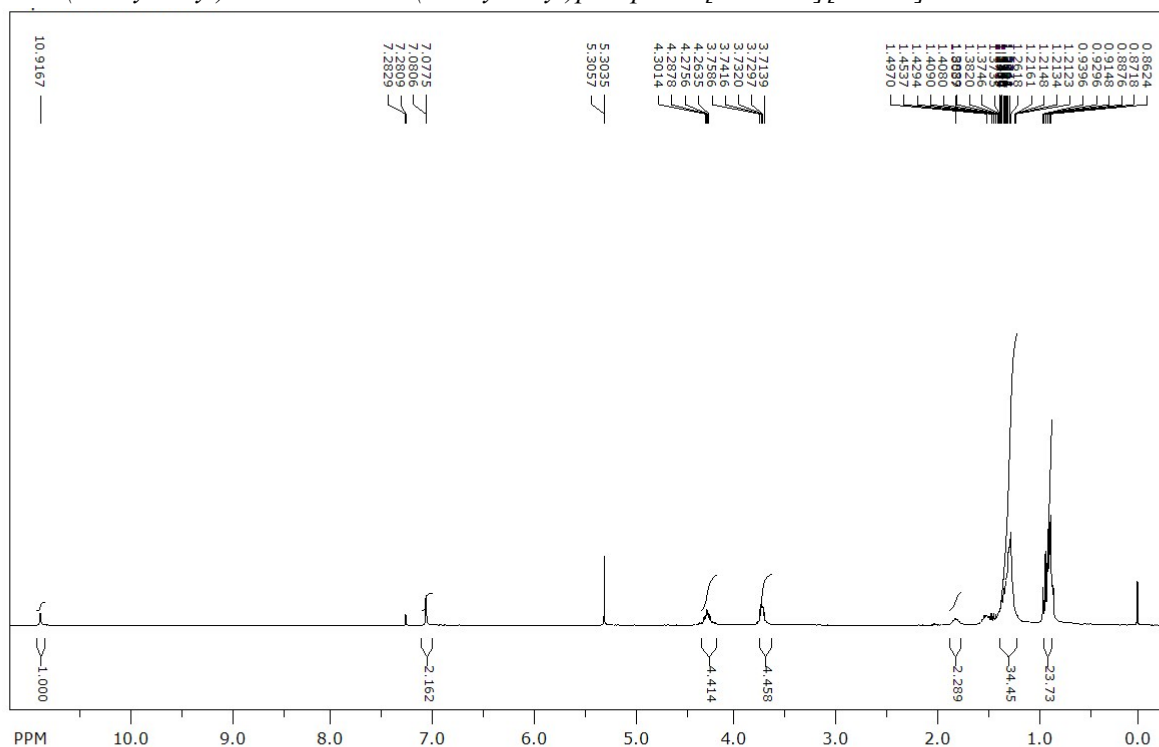
Peak at 5.30 ppm is attributed to residual DCM.

1,3-Didecylimidazolium bis(2-ethylhexyl)phosphate [DDIM][DEHP]



Peak at 5.30 ppm is attributed to residual DCM.

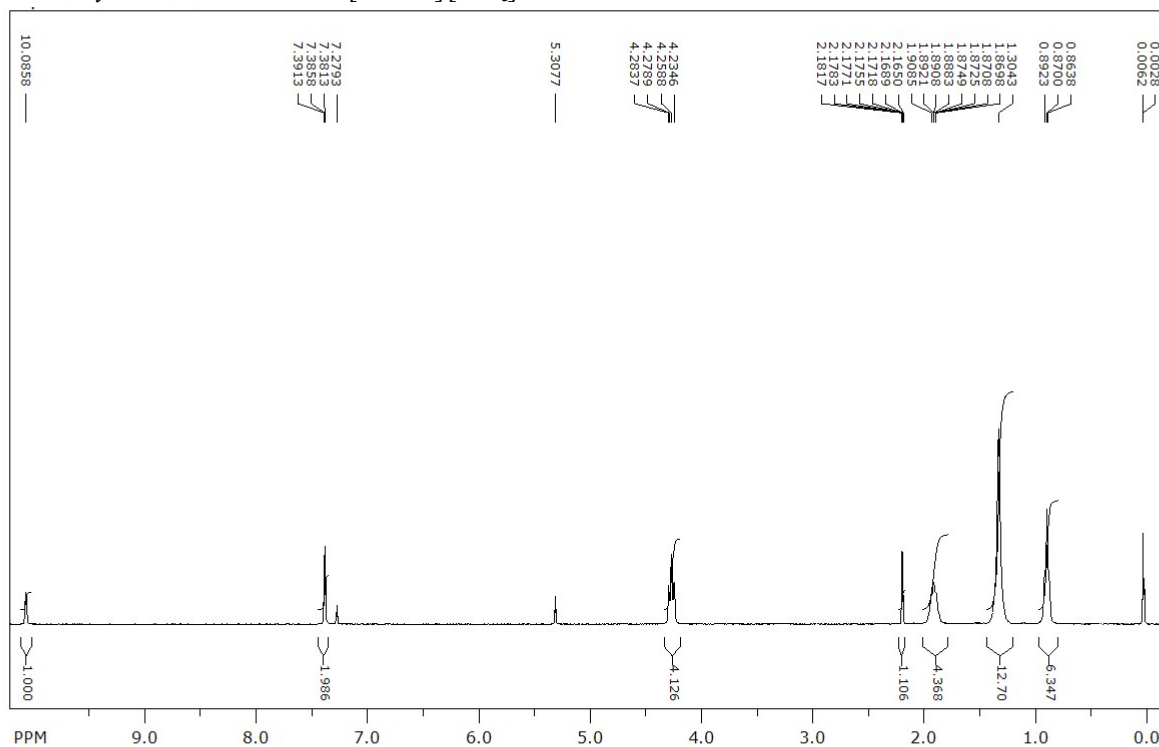
1,3-Bis(2-ethylhexyl)imidazolium bis(2-ethylhexyl)phosphate [EhEhIM][DEHP]



Peak at 5.30 ppm is attributed to residual DCM.

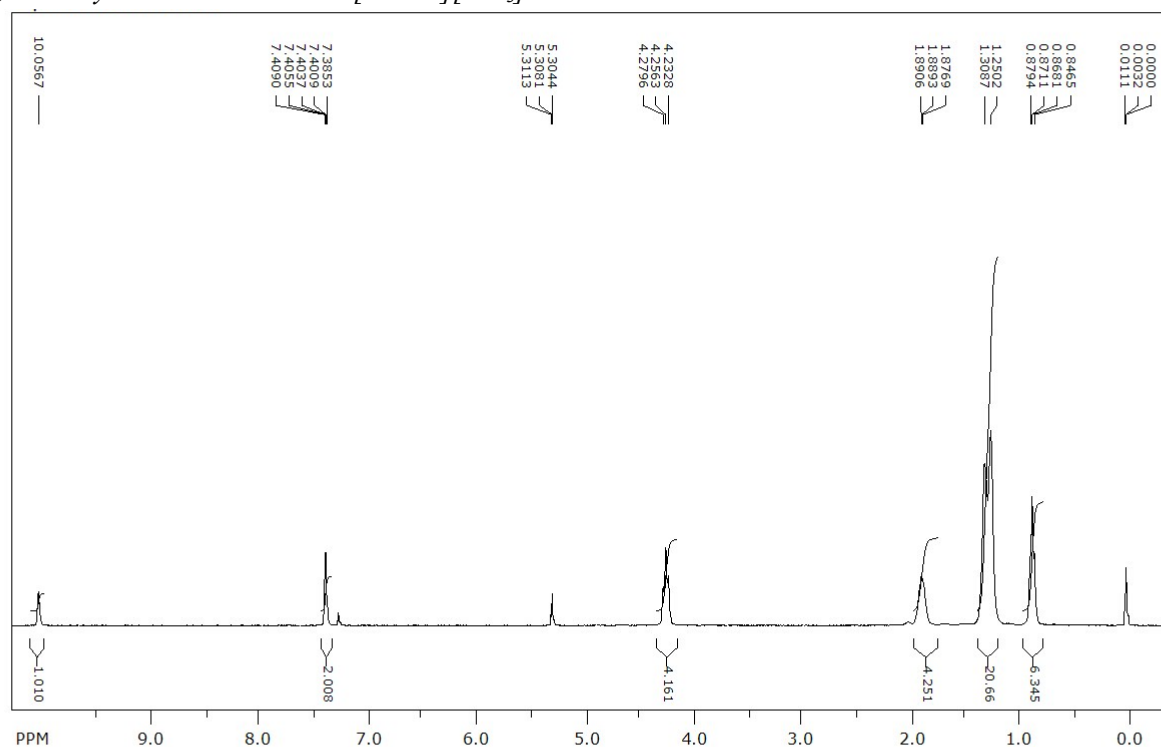
Nitrate ILs

1,3-Dihexylimidazolium nitrate[HHIM][NO₃]



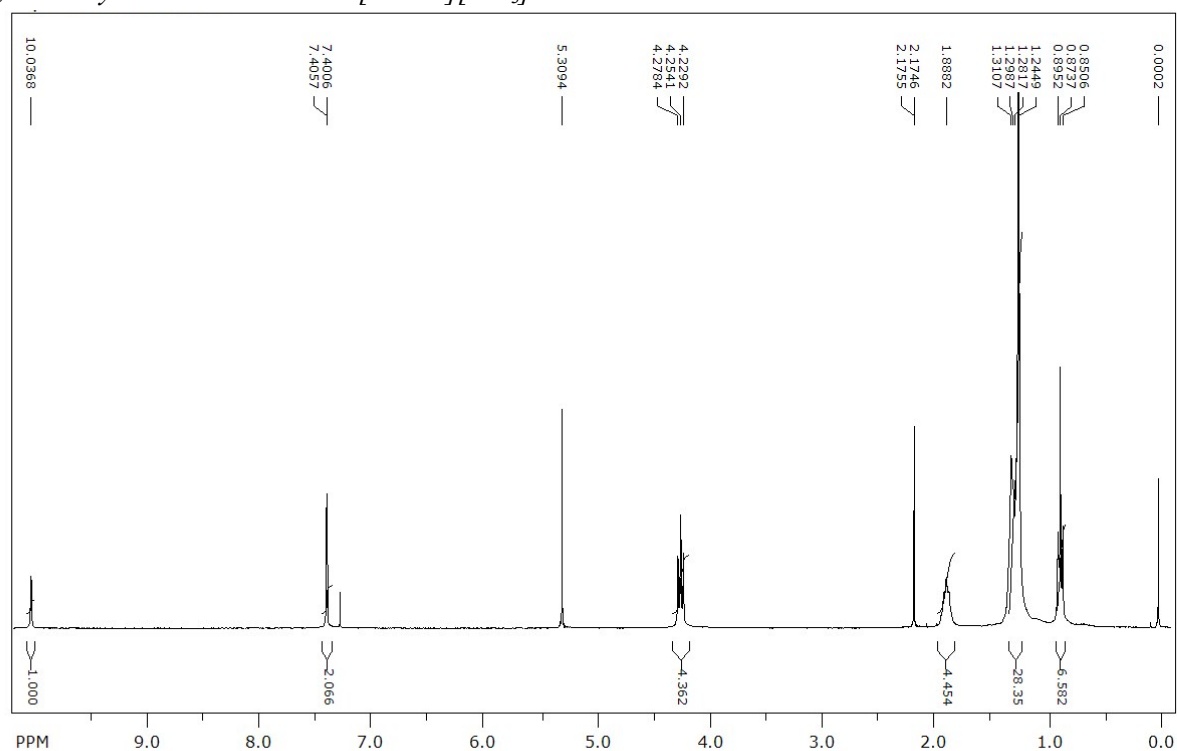
Peak at 5.30 ppm is attributed to residual DCM, peak at 2.17 ppm is attributed to acetone.

1,3-Dioctylimidazolium nitrate [OOIM][NO₃]



Peak at 5.30 ppm is attributed to residual DCM.

1,3-Didecylimidazolium nitrate [DDIM][NO₃]



Peak at 5.30 ppm is attributed to residual DCM, peak at 2.17 ppm is attributed to acetone.

1,3-Bis(2-ethylhexyl)imidazolium nitrate [EhEhIM][NO₃]

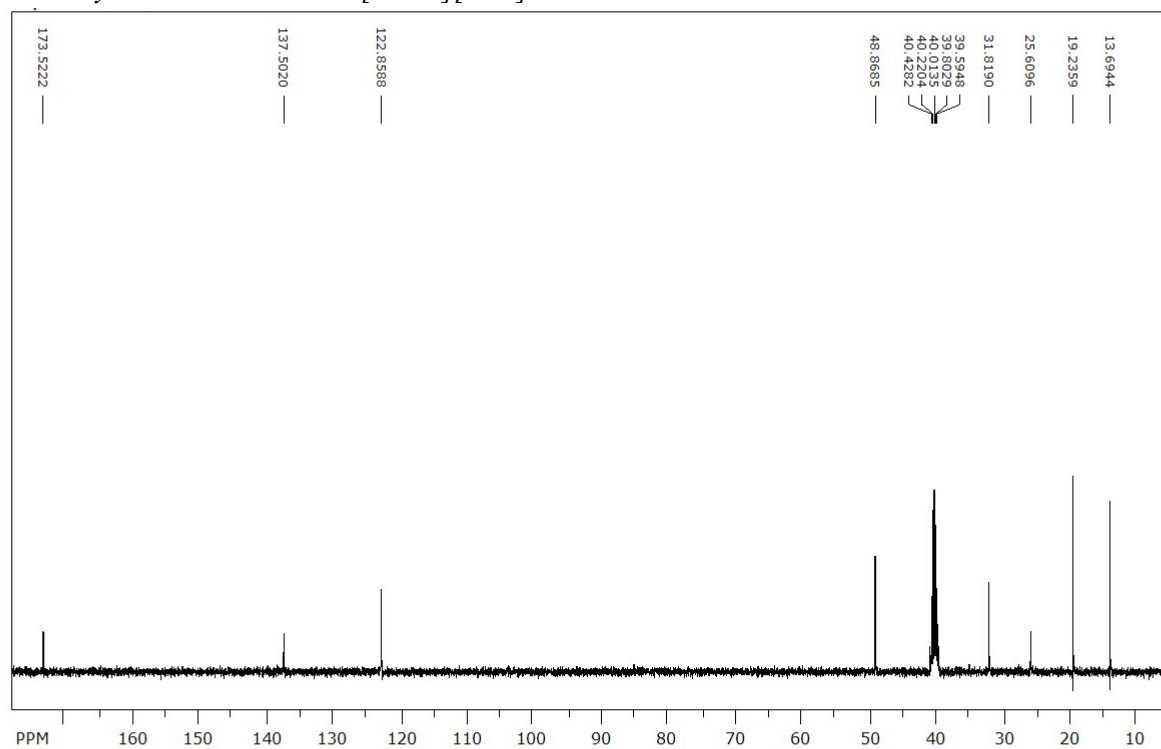


Acetate ILs

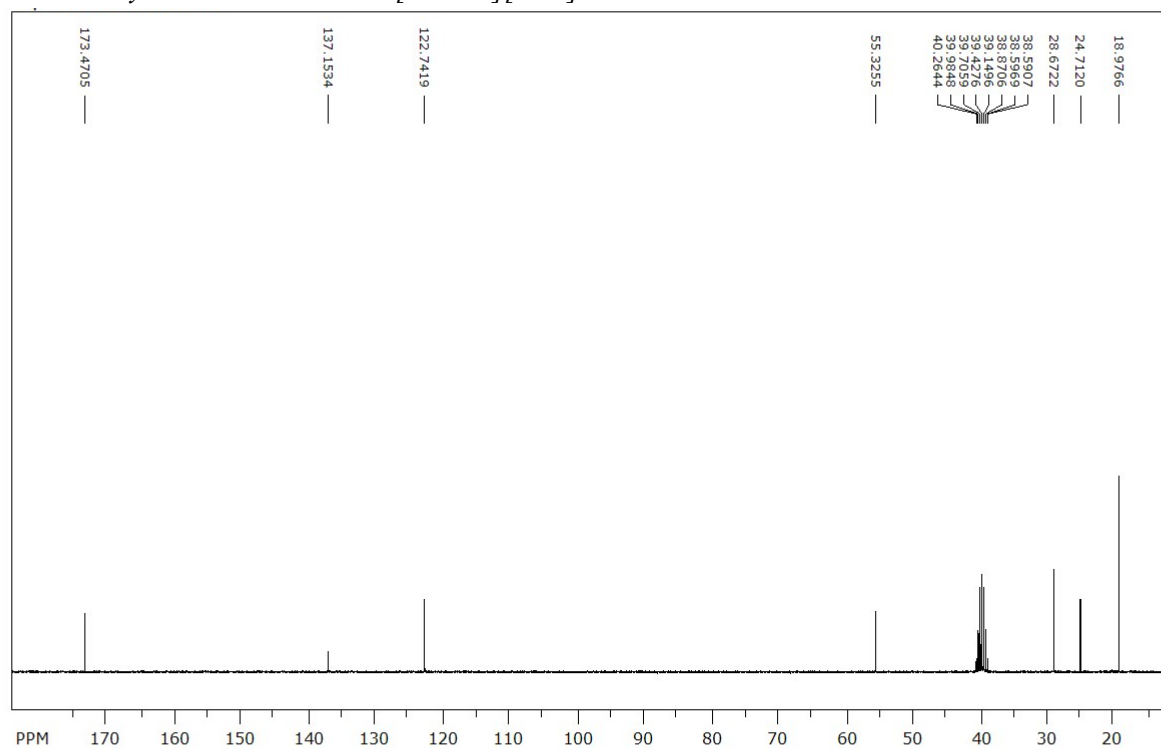
15.0806 —
24.8535 —
38.6479
38.7270
38.7341
38.7420
38.7601
40.0391
40.3159
44.0220
122.0186 —
136.1719 —
173.0443 —

PPM

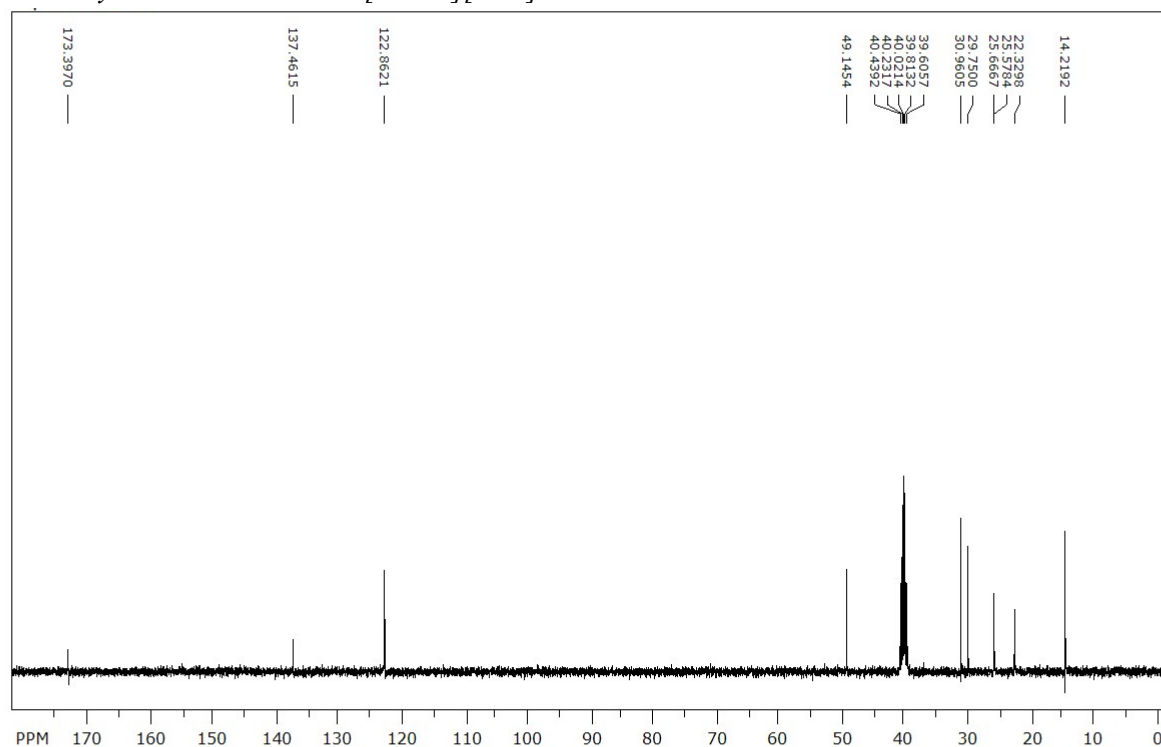
1,3-Dibutylimidazolium acetate [BBIM][AcO]



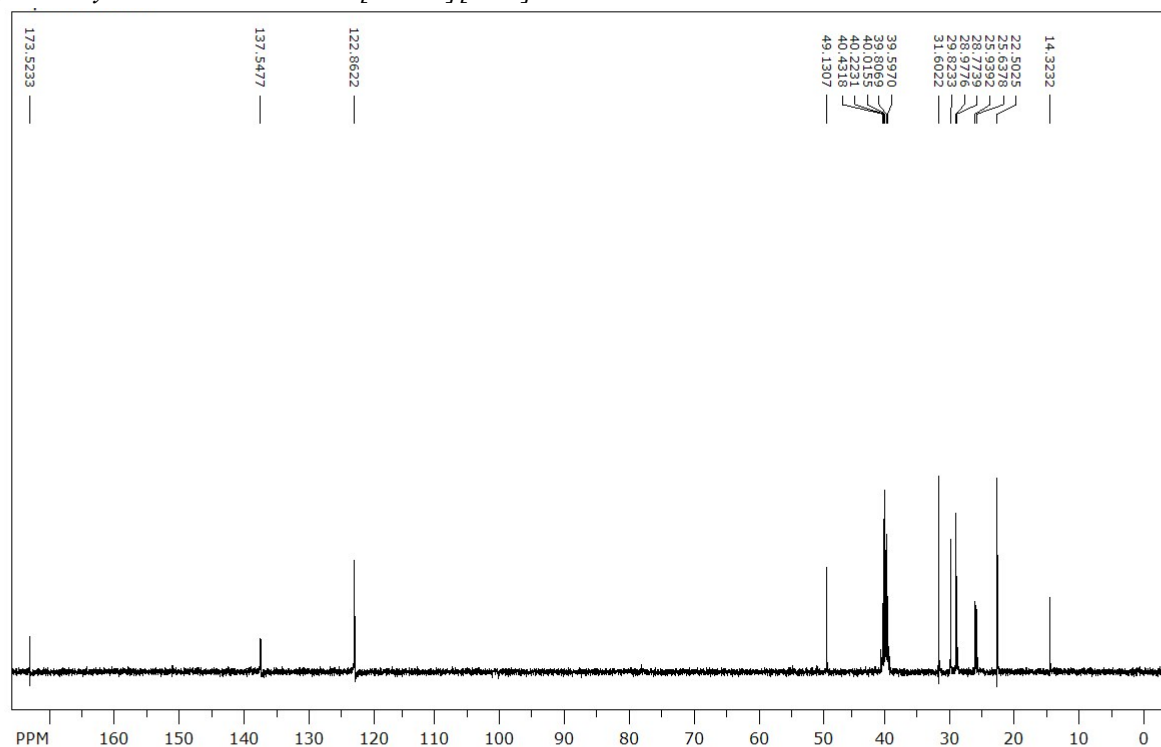
1,3-Diisobutylimidazolium acetate [iBiBIM][AcO]



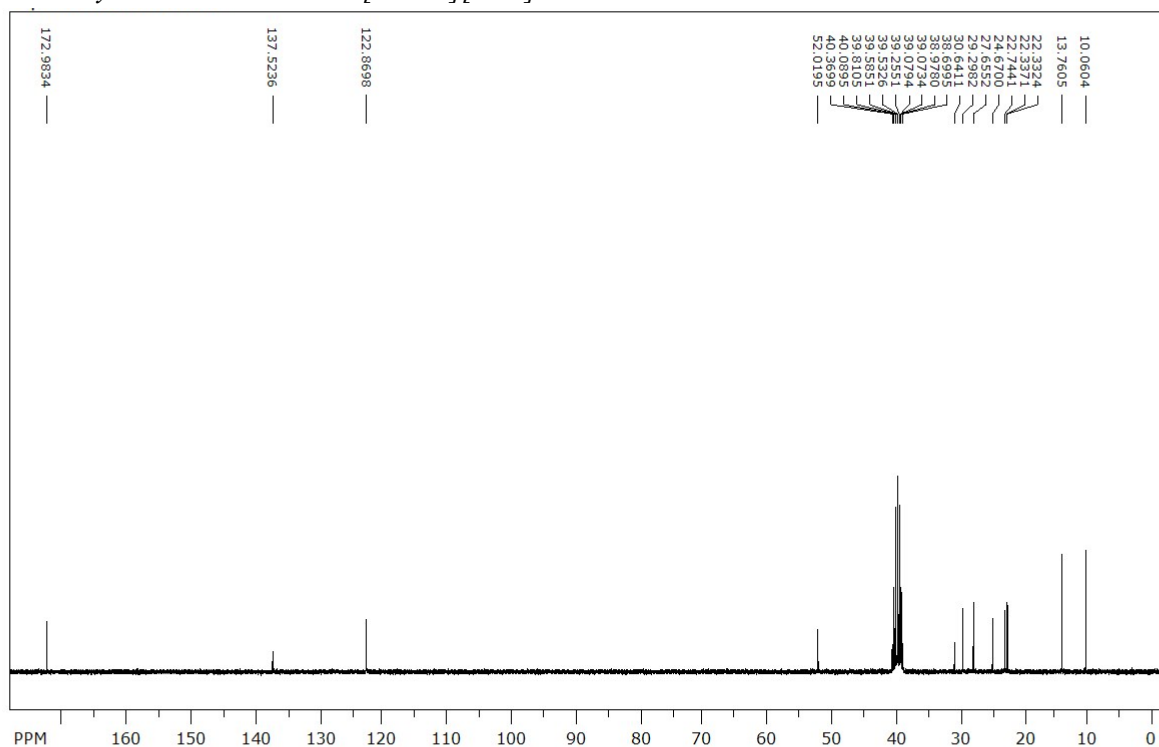
1,3-Dihexylimidazolium acetate [HHIM][AcO]



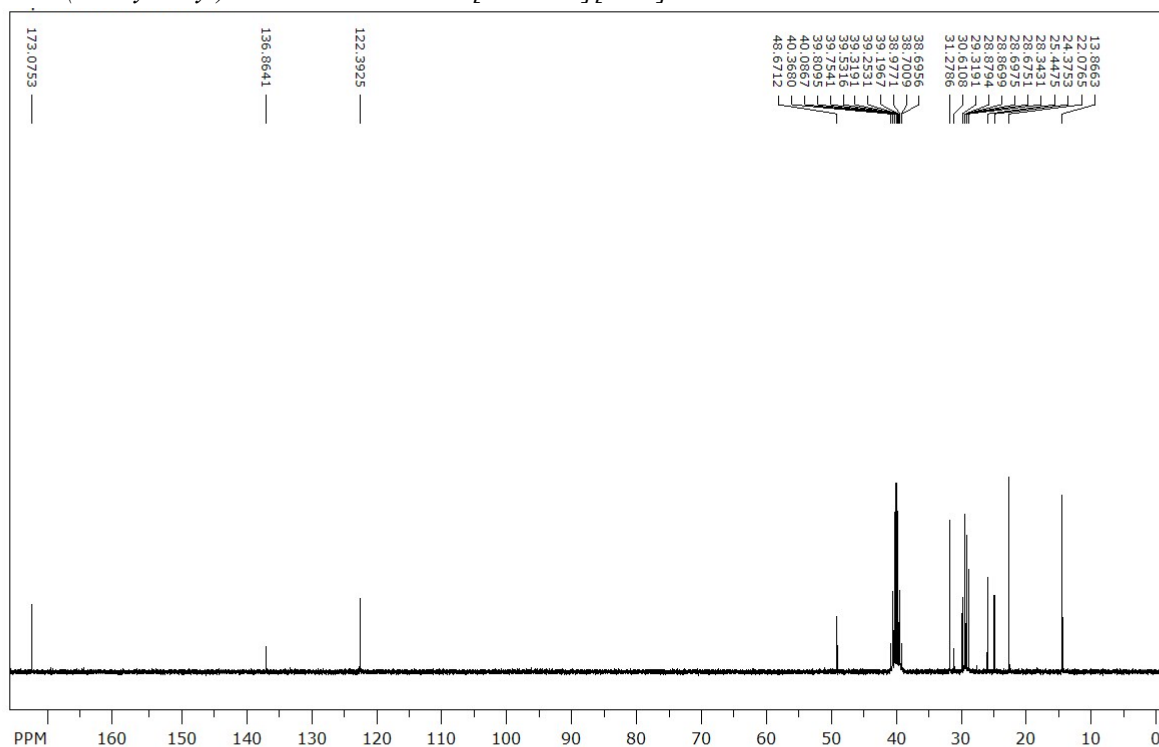
1,3-Dioctylimidazolium acetate [OOIM][AcO]



1,3-Didecylimidazolium acetate [DDIM][AcO]

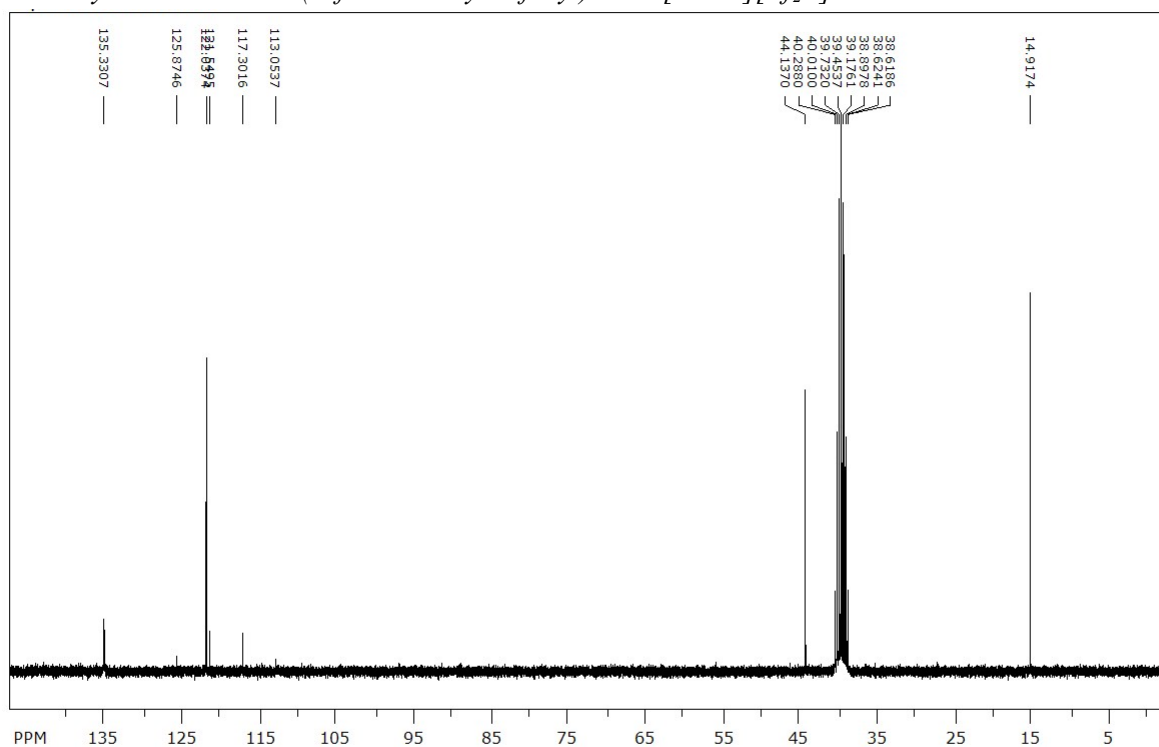


1,3-Bis(2-ethylhexyl)imidazolium acetate [EhEhIM][AcO]

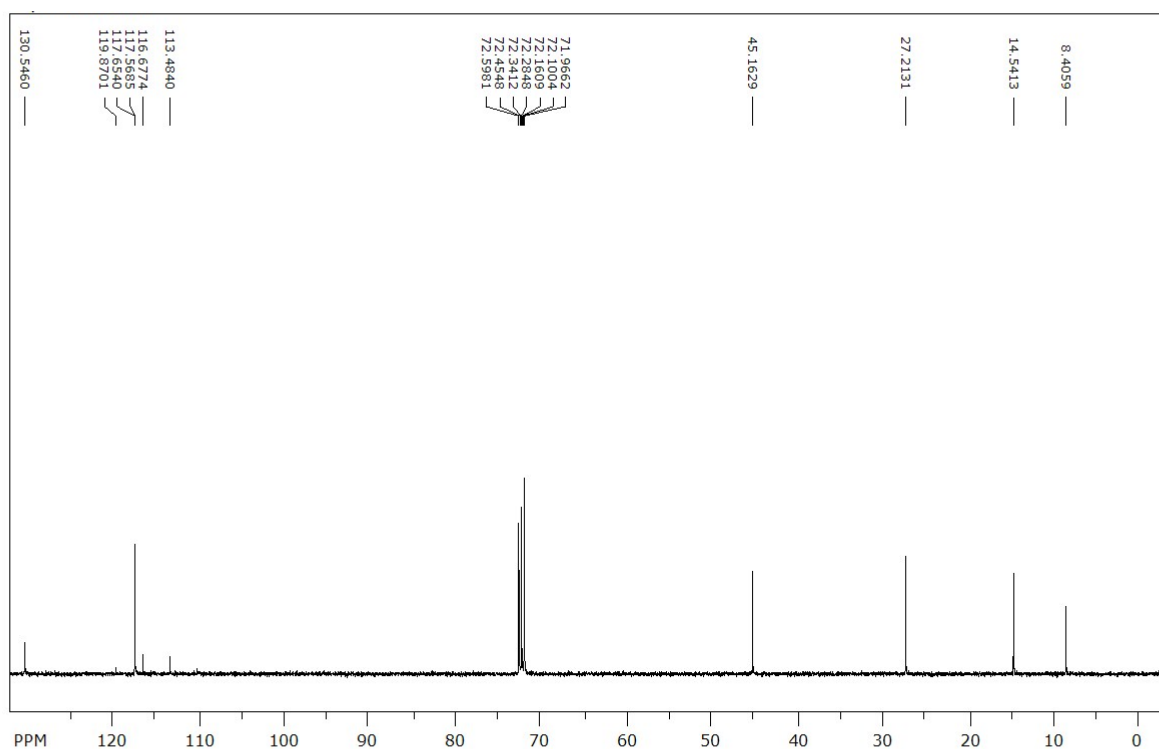


Bis(trifluoromethylsulfonyl)imide ILs

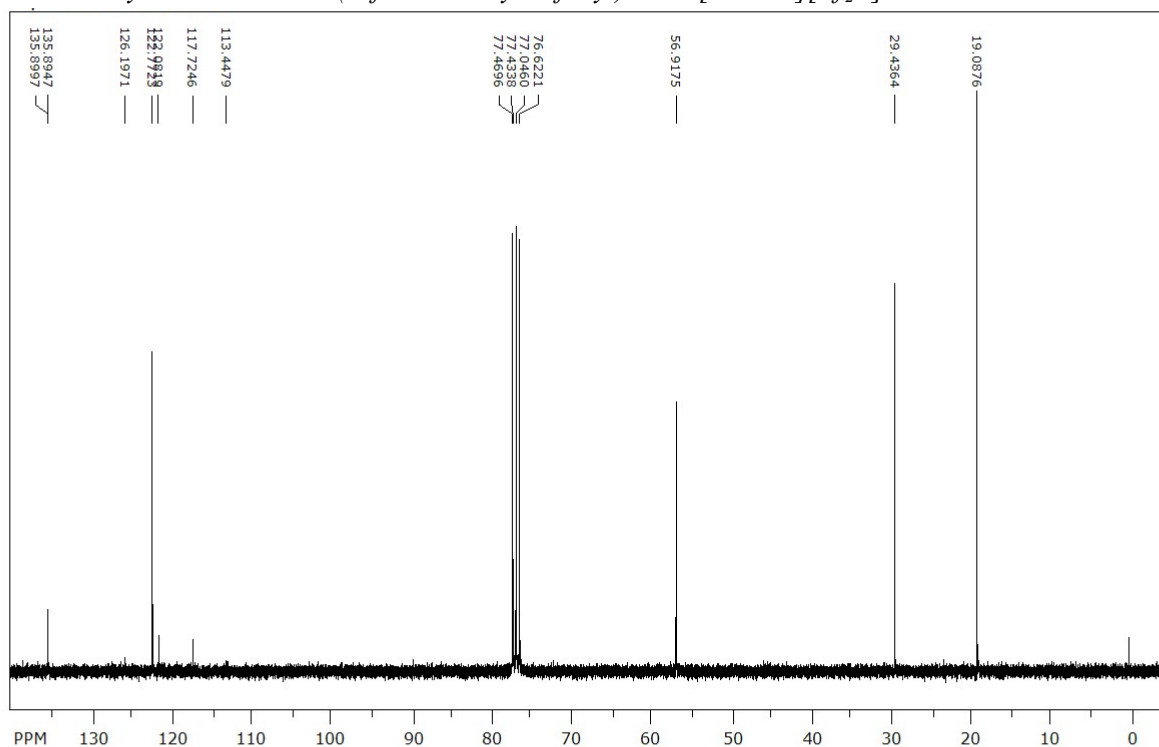
1,3-Diethylimidazolium bis(trifluoromethylsulfonyl)imide [EEIM][Tf₂N]



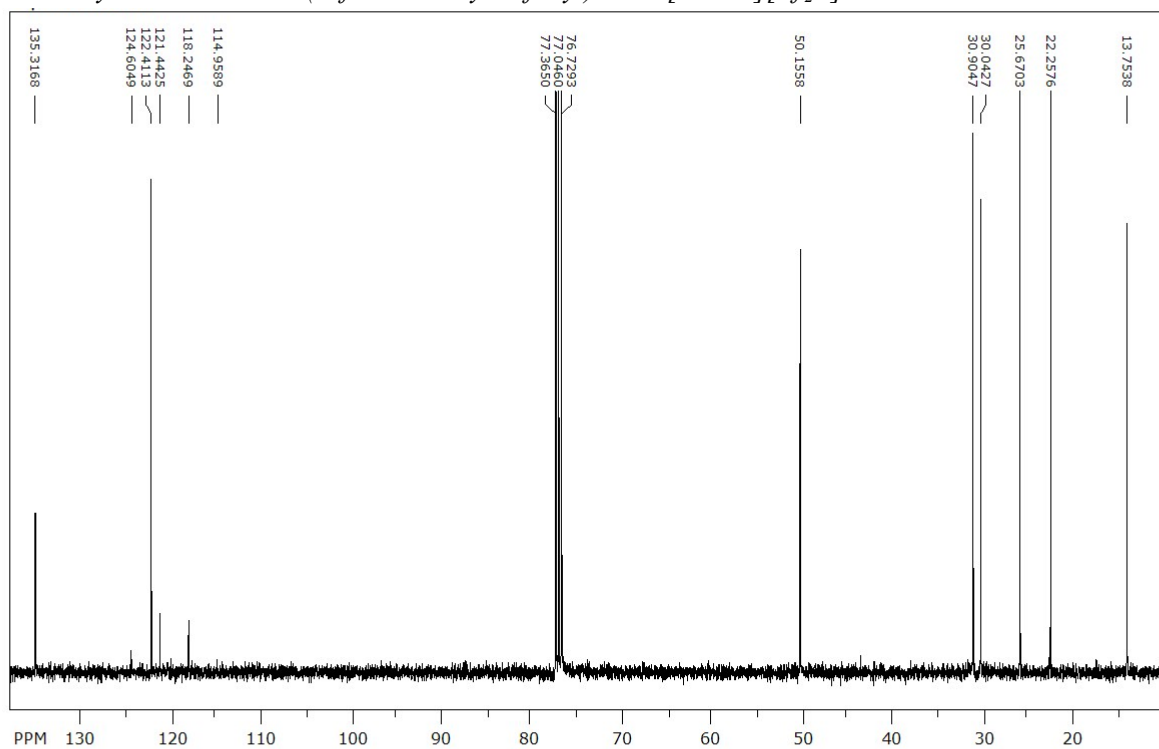
1,3-Dibutylimidazolium bis(trifluoromethylsulfonyl)imide [BBIM][Tf₂N]



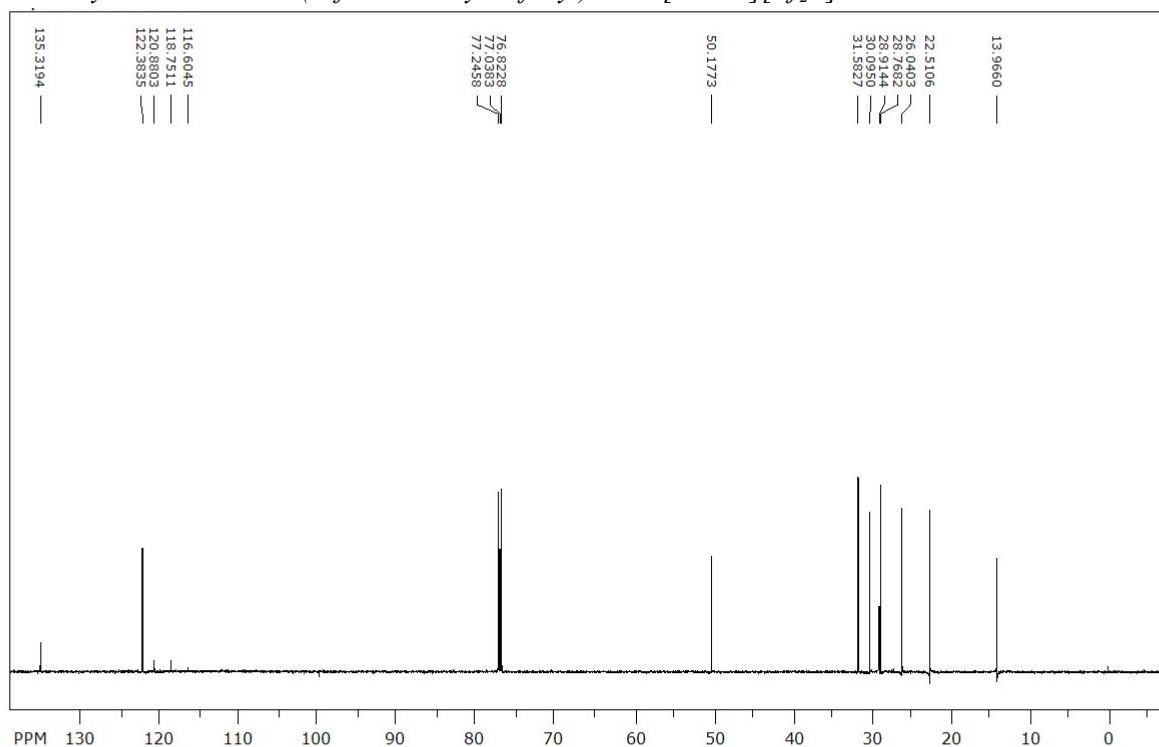
1,3-Diisobutylimidazolium bis(trifluoromethylsulfonyl)imide [iBiBIM][Tf₂N]



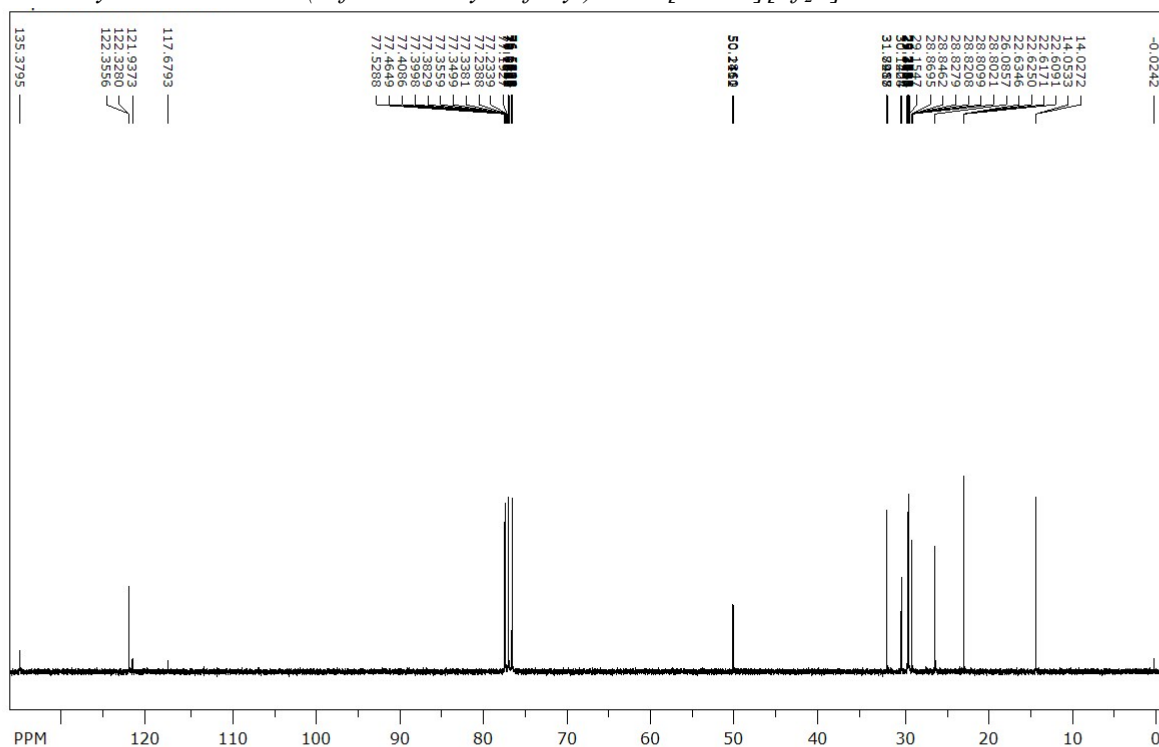
1,3-Dihexylimidazolium bis(trifluoromethylsulfonyl)imide [HHIM][Tf₂N]



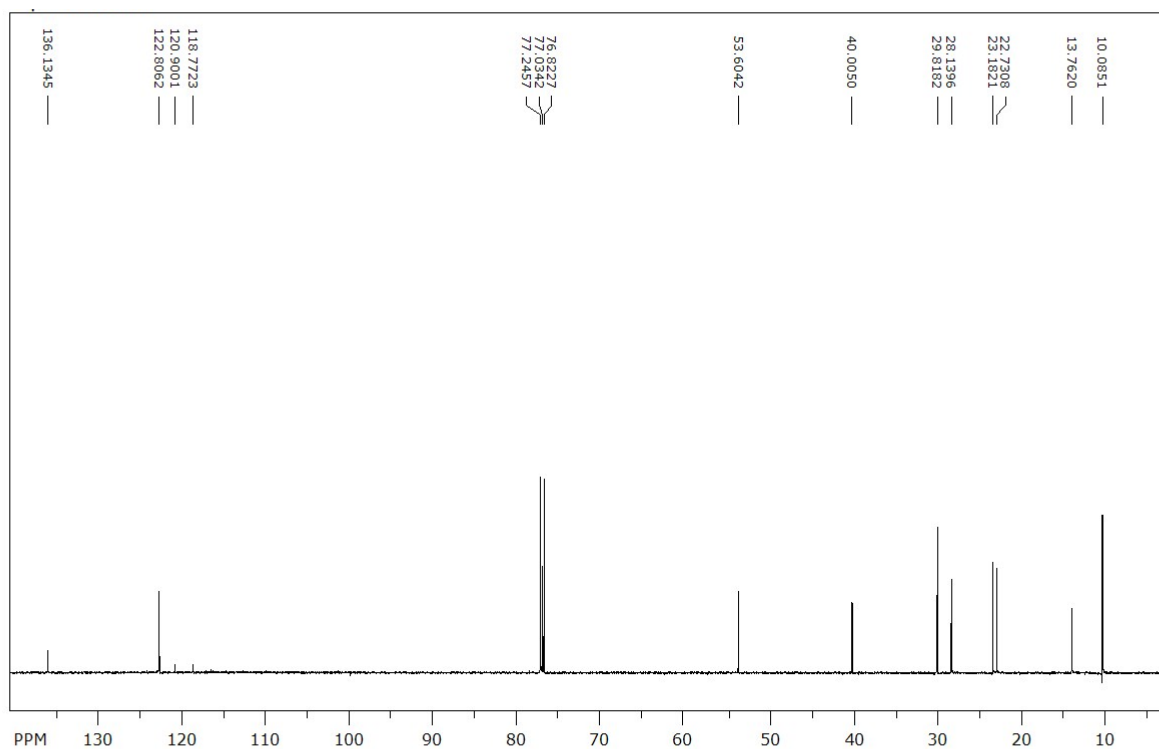
1,3-Dioctylimidazolium bis(trifluoromethylsulfonyl)imide [OOIM][Tf₂N]



1,3-Didecylimidazolium bis(trifluoromethylsulfonyl)imide [DDIM][Tf₂N]

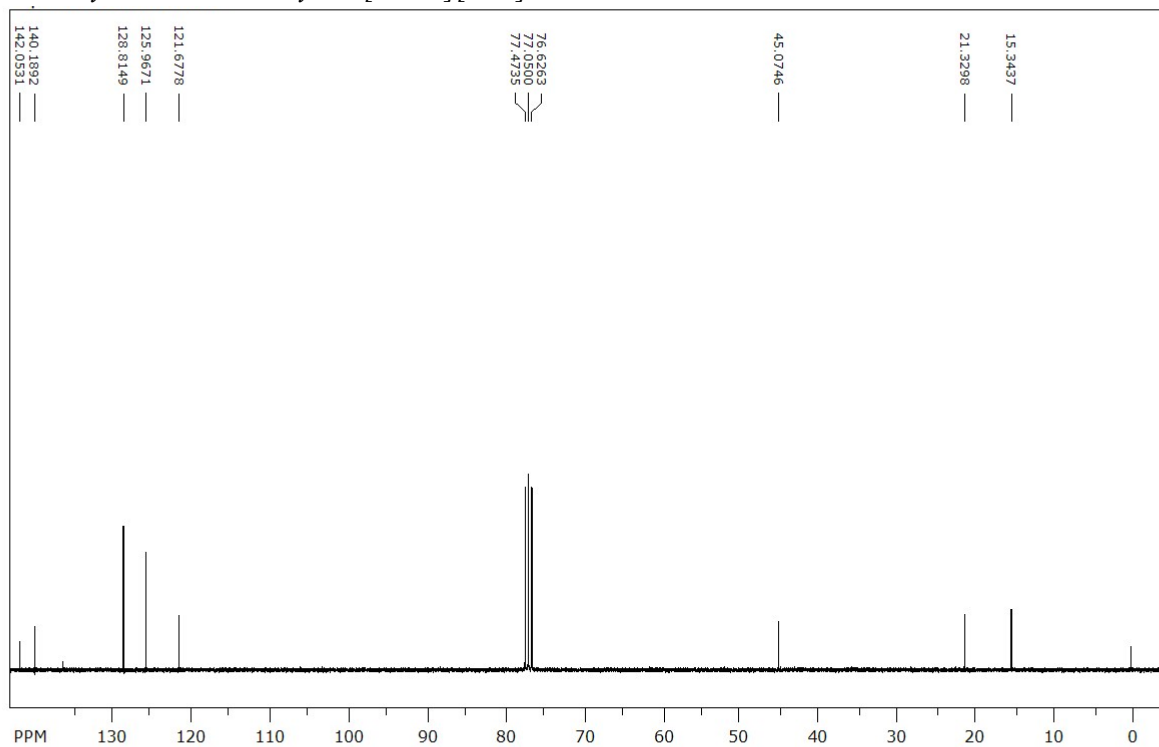


1,3-Bis(2-ethylhexyl)imidazolium bis(trifluoromethylsulfonyl)imide [EhEhIM][Tf₂N]

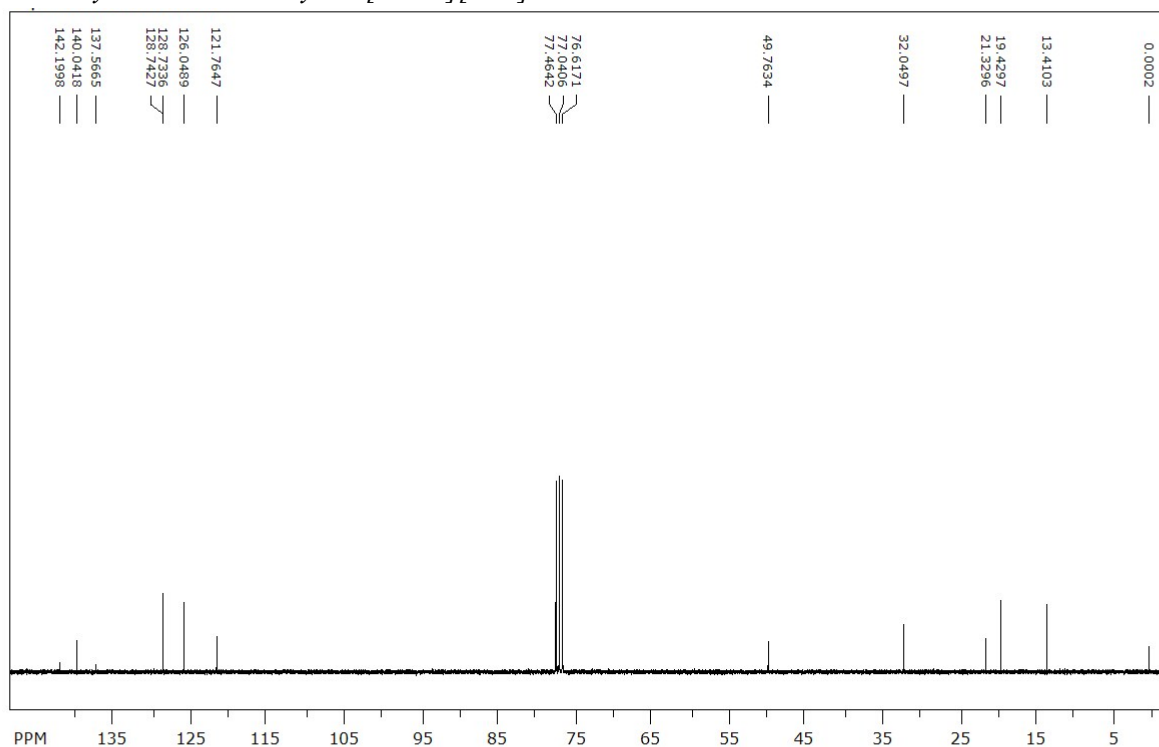


Tosylate ILs

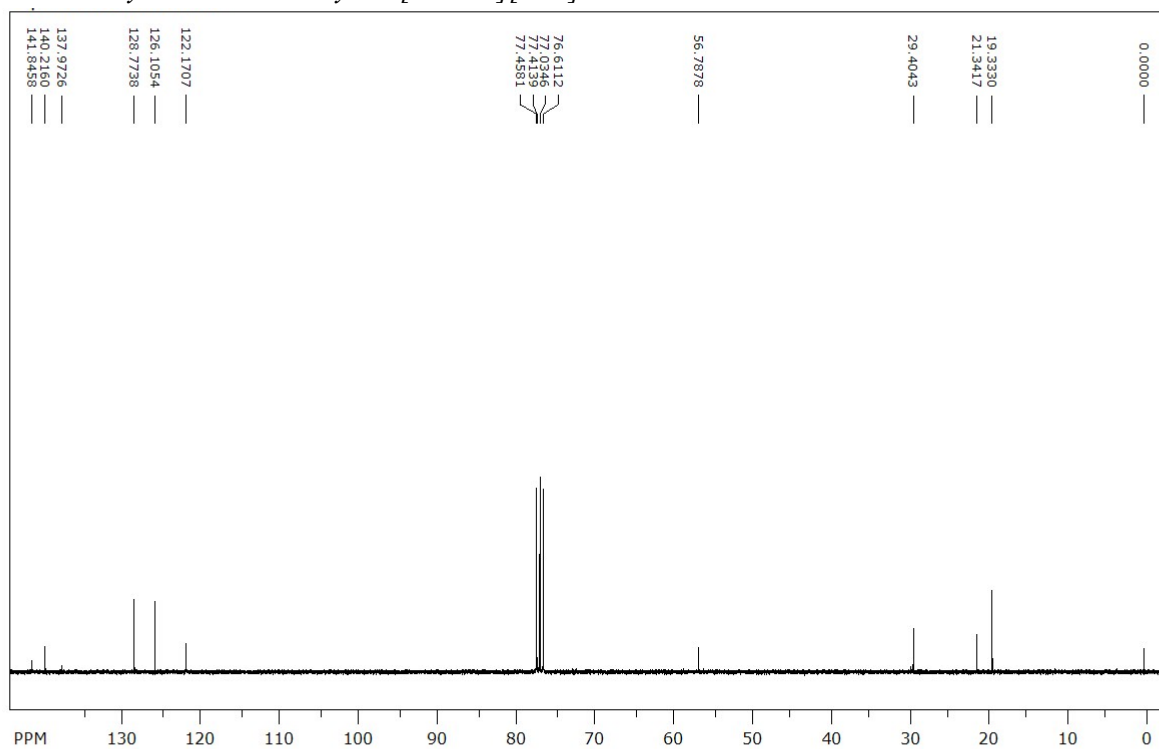
1,3-Diethylimidazolium tosylate [EEIM][OTs]



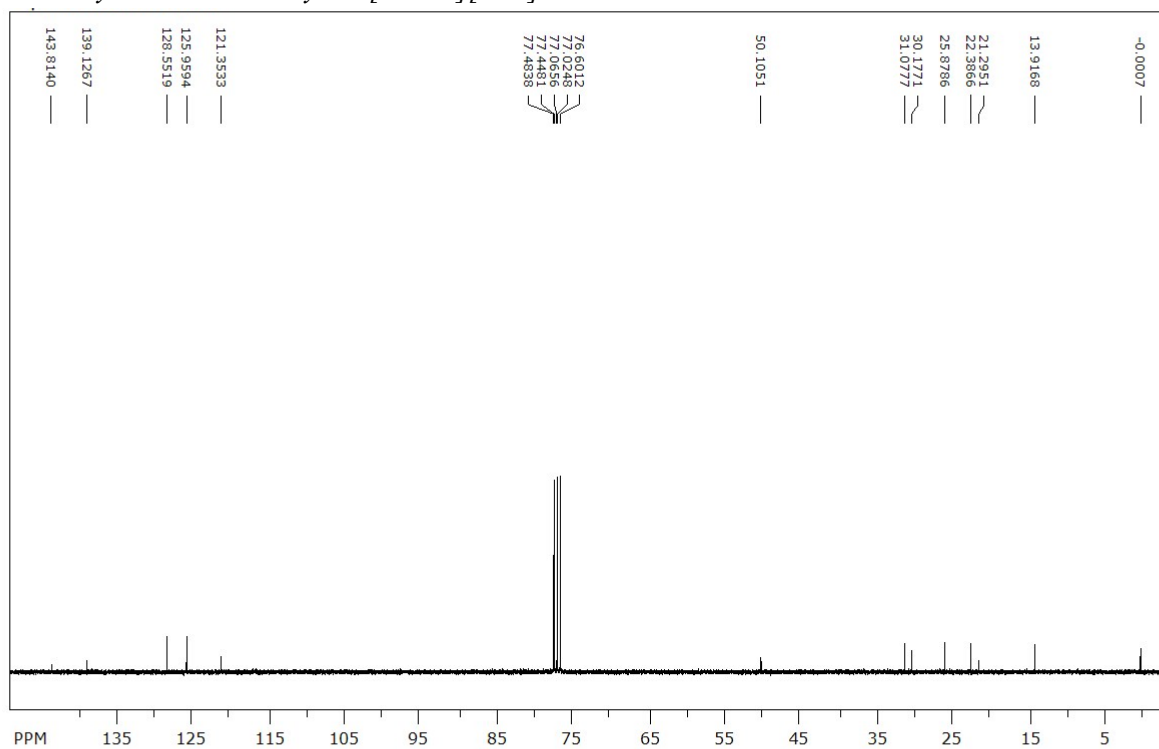
1,3-Dibutylimidazolium tosylate [BBIM][OTs]



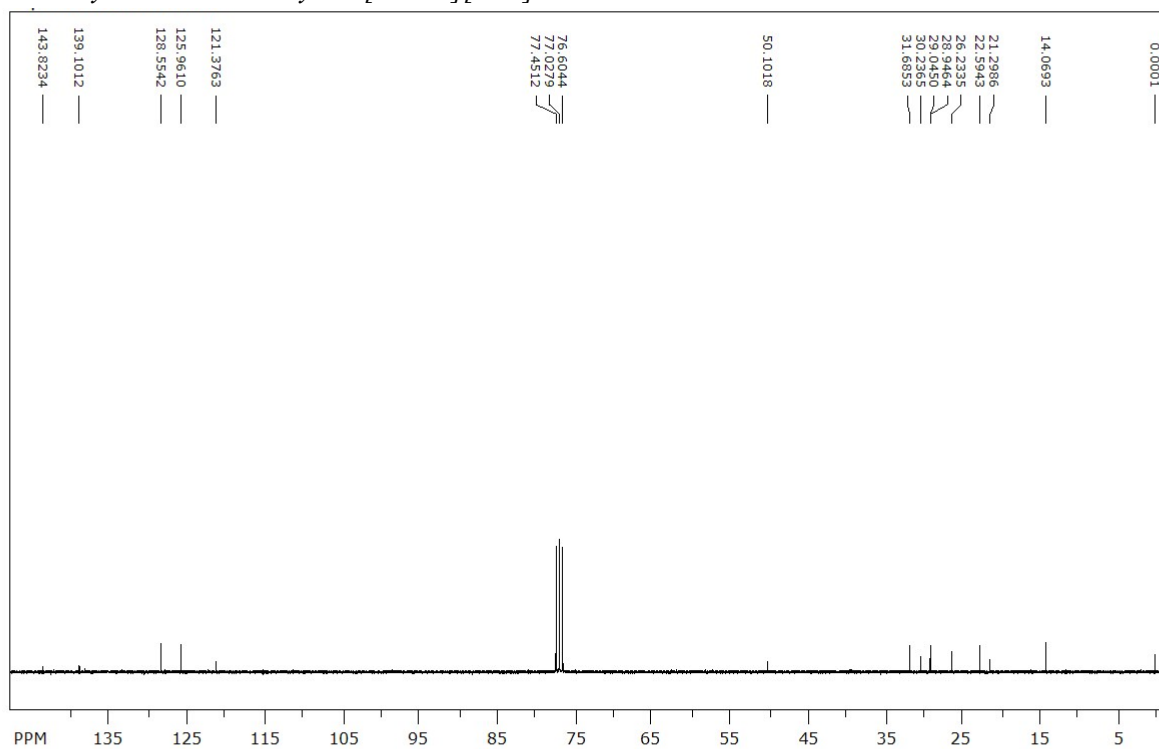
1,3-Diisobutylimidazolium tosylate [iBiBIM][OTs]



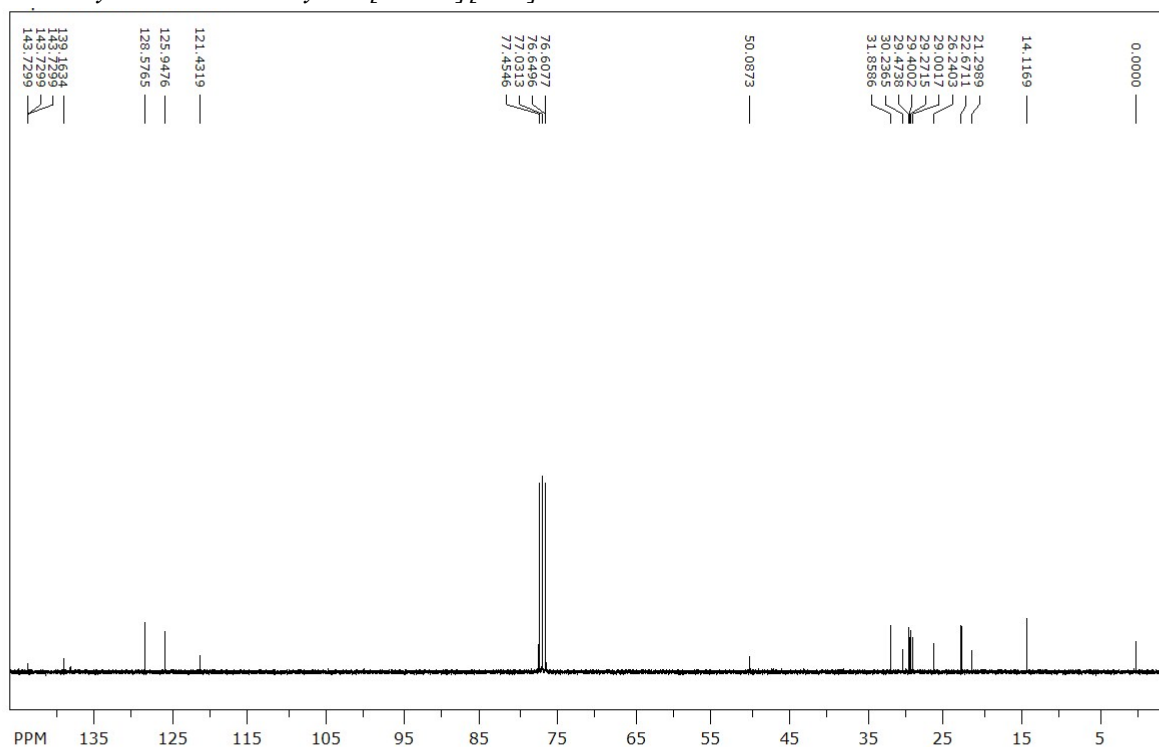
1,3-Dihexylimidazolium tosylate [HHIM][OTs]



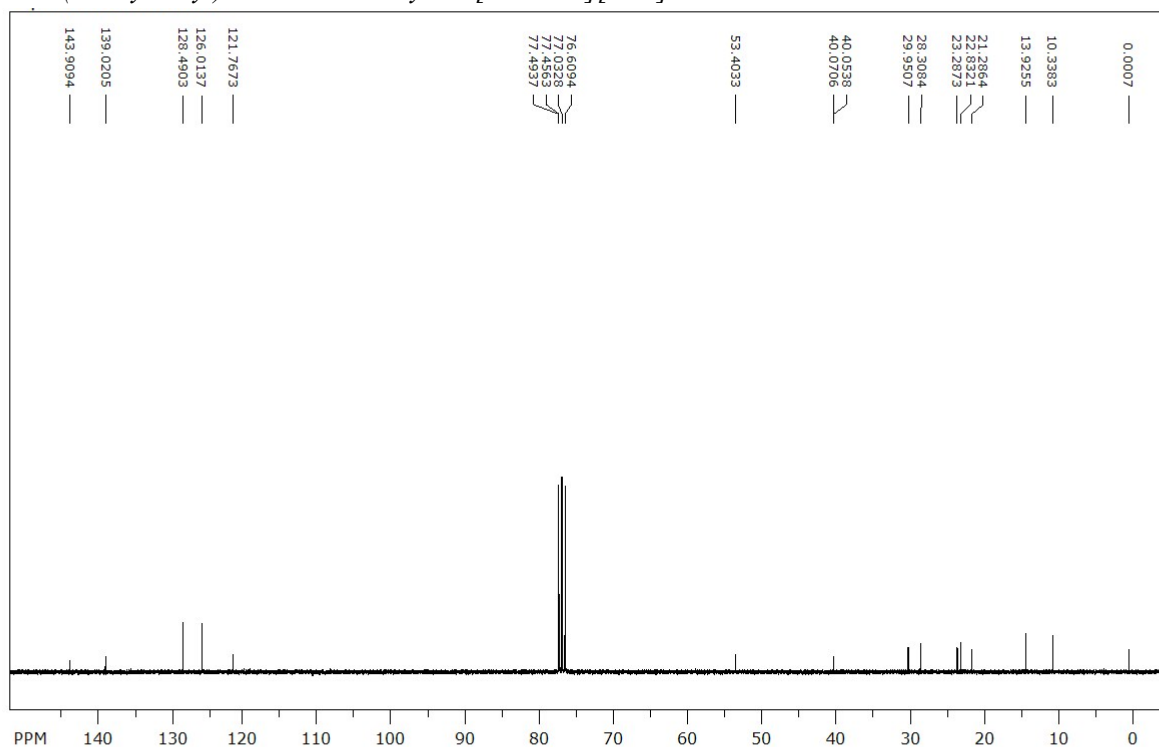
1,3-Dioctylimidazolium tosylate [OOIM][OTs]



1,3-Didecylimidazolium tosylate [DDIM][OTs]

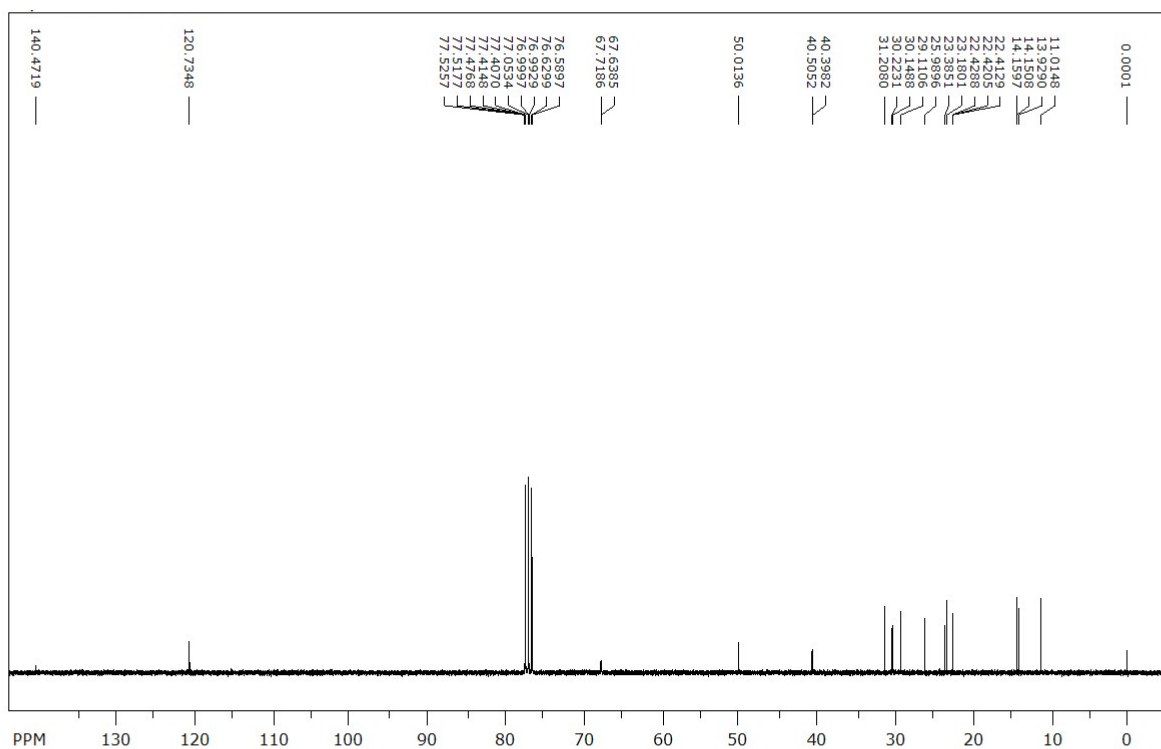


1,3-bis(2-ethylhexyl)imidazolium tosylate [EhEhIM][OTs]

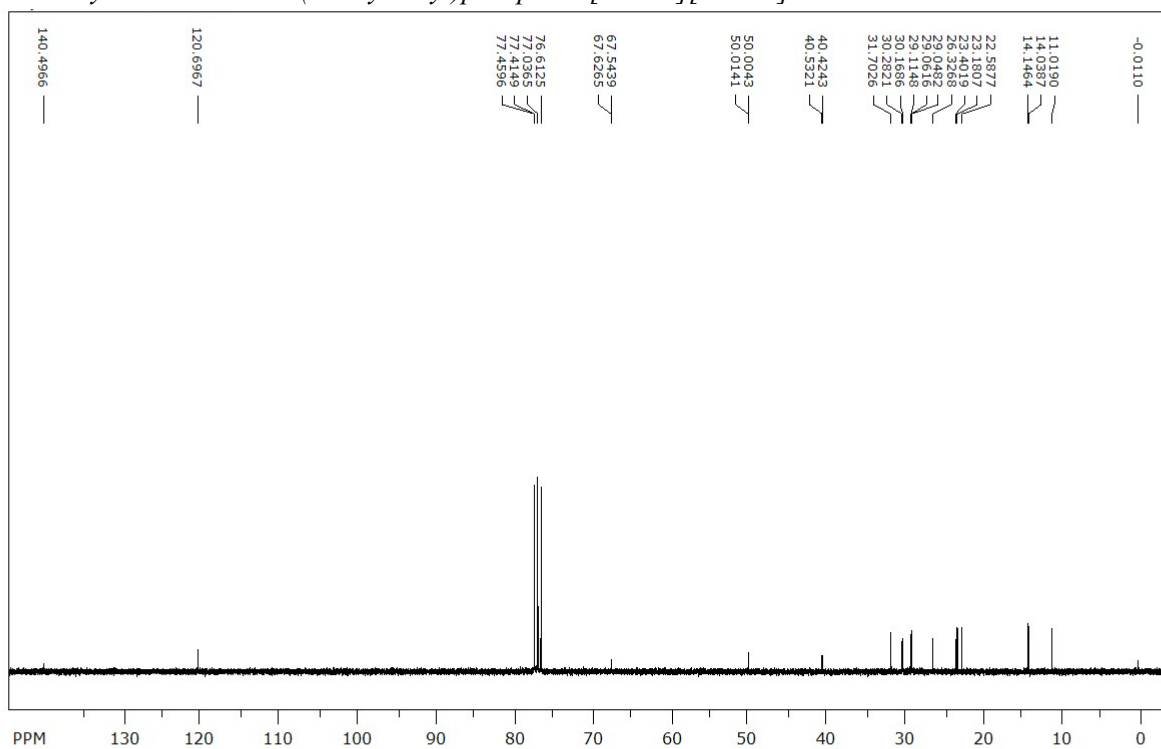


Bis(2-ethylhexyl)phosphate ILs

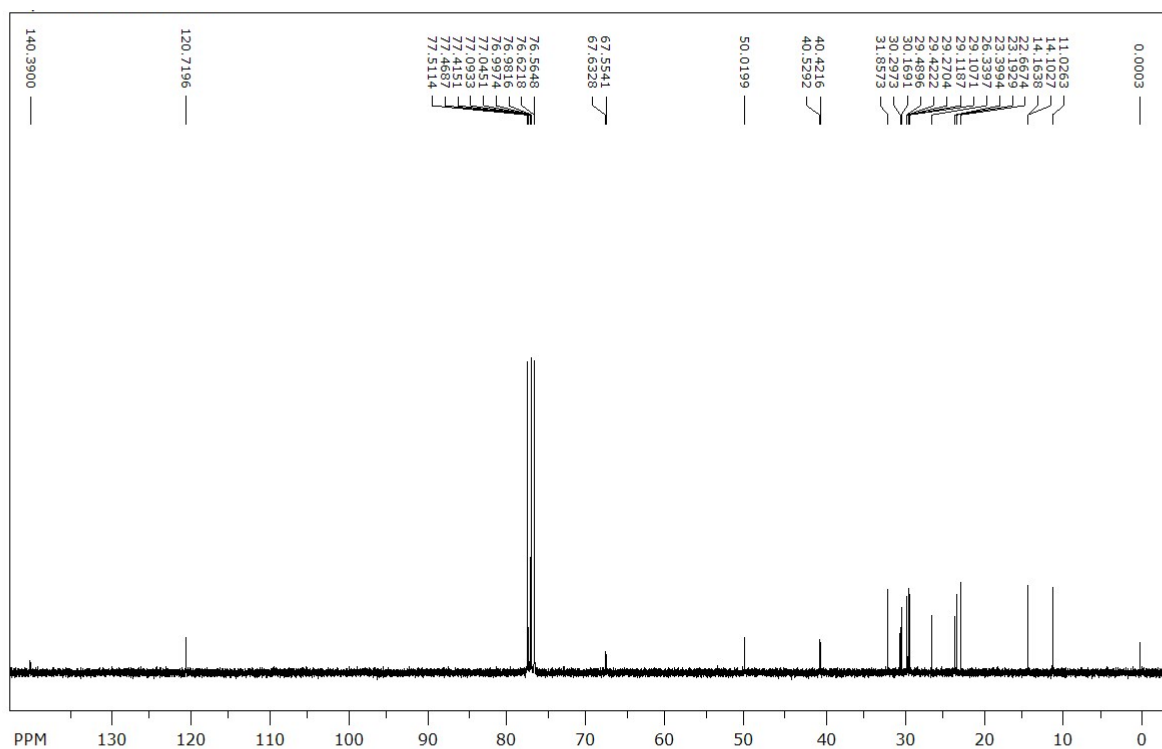
1,3-Dihexylimidazolium bis(2-ethylhexyl)phosphate [HHIM][DEHP]



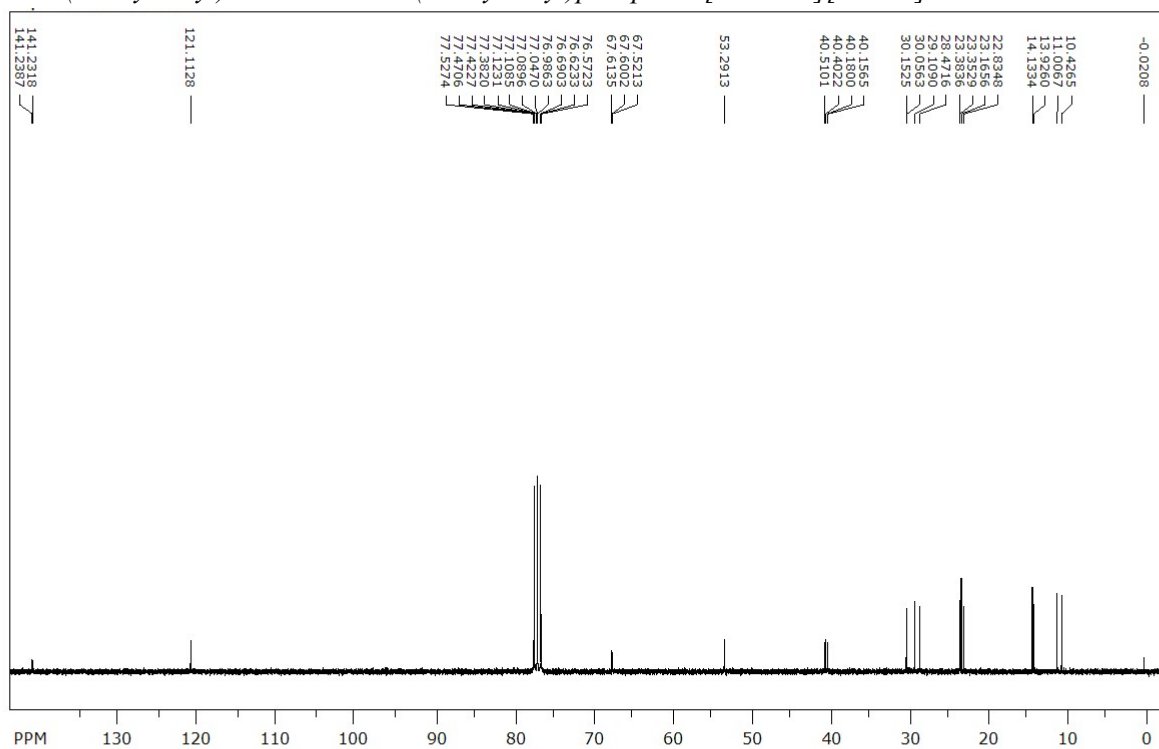
1,3-Dioctylimidazolium bis(2-ethylhexyl)phosphate [OOIM][DEHP]



1,3-Didecylimidazolium bis(2-ethylhexyl)phosphate [DDIM][DEHP]

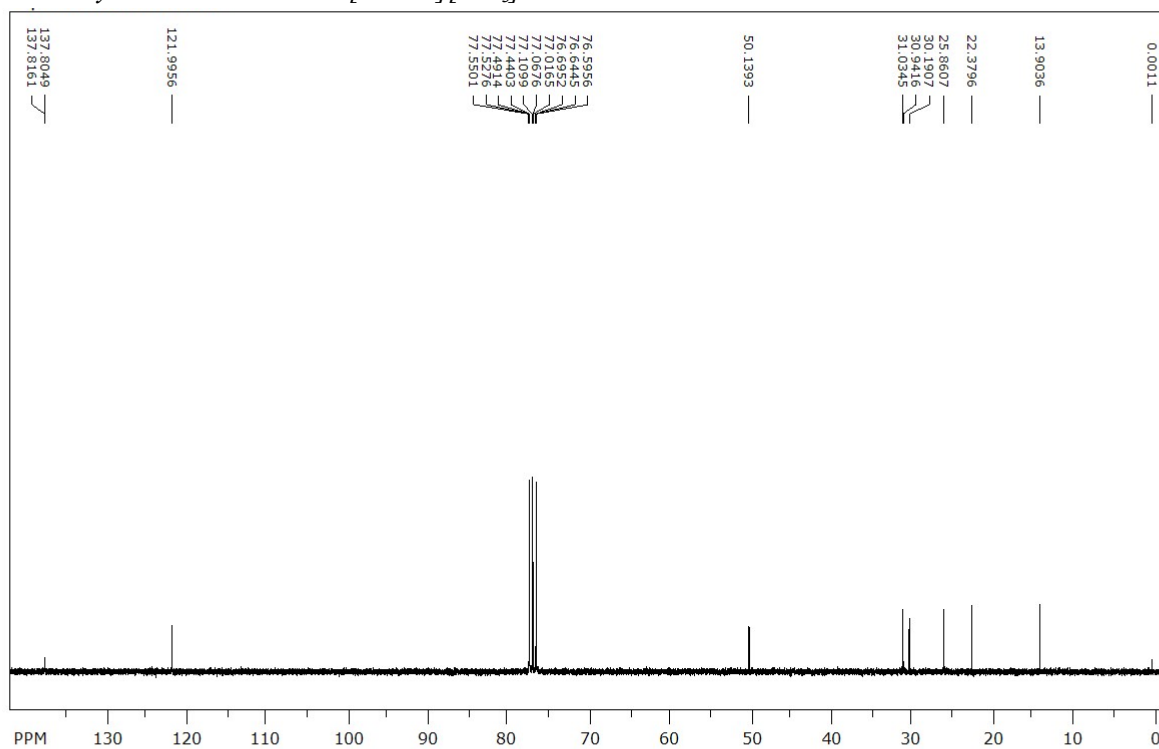


1,3-Bis(2-ethylhexyl)imidazolium bis(2-ethylhexyl)phosphate [EhEhIM][DEHP]

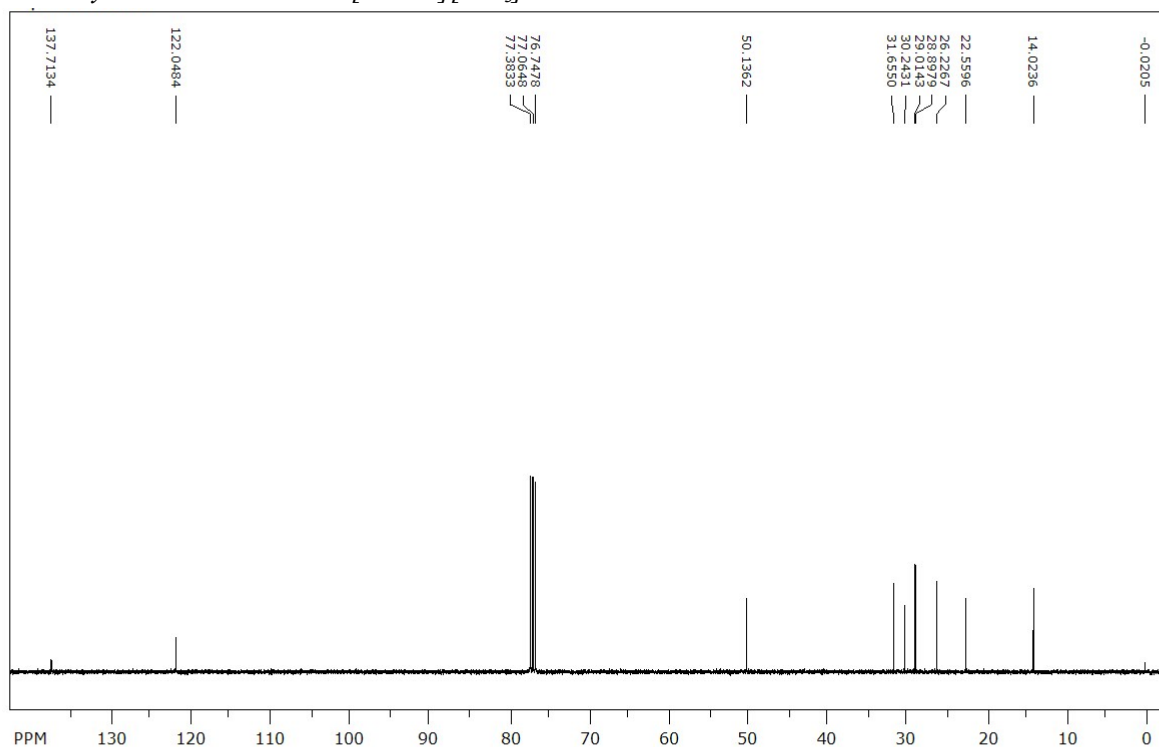


Nitrate ILs

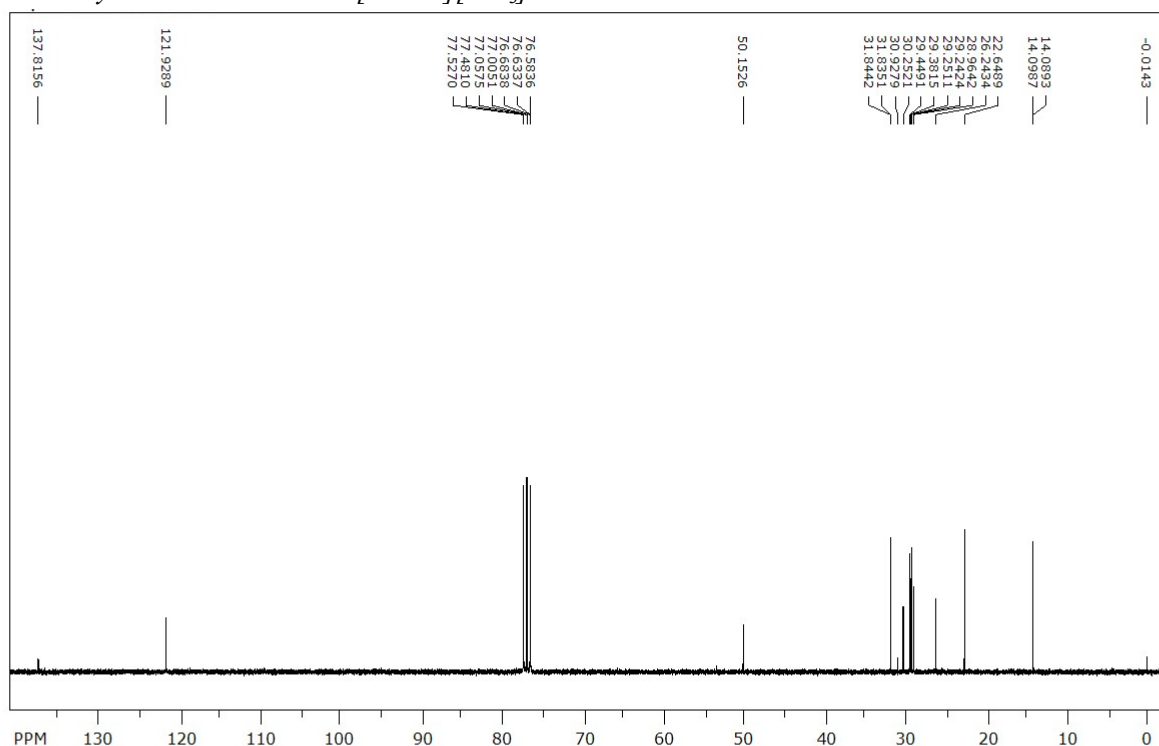
1,3-Dihexylimidazolium nitrate[HHIM][NO₃]



1,3-Dioctylimidazolium nitrate [OOIM][NO₃]



1,3-Didecylimidazolium nitrate [DDIM][NO₃]



1,3-Bis(2-ethylhexyl)imidazolium nitrate [EhEhIM][NO₃]

