

## Molecular interactions between ammonium-based ionic liquids and molecular solvents: current progress and challenges

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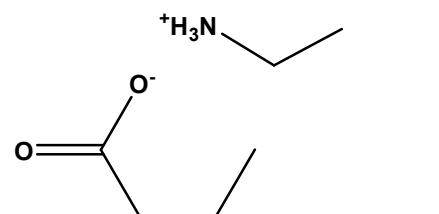
**Table 1S. Name, abbreviation and chemical structure of ammonium-based ionic liquids:**

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Name of the ionic liquid	Abbreviation	Structure
Ethylammonium nitrate	[EAN]	
N-propylammonium nitrate	[PAN]	
N-butylammonium nitrate	[BAN]	
Methylammonium formate	[MAF]	
Ethylammonium formate	[EAF]	
Propylammonium formate	[PAF]	
Butylammonium formate	[BAF]	
Pentylammonium formate	[PeAF]	
Ethylammonium propionate	[EAP]	

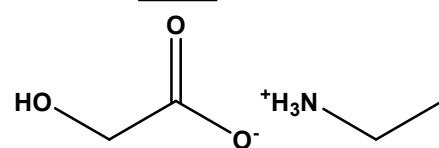
Ethylammonium butyrate

[EAB]



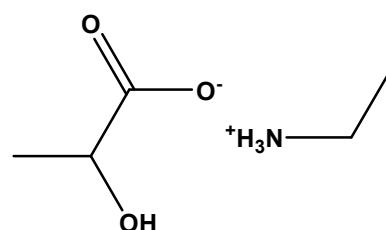
Ethylammonium glycolate

[EAG]



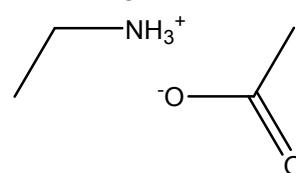
Ethylammonium lactate

[EAL]



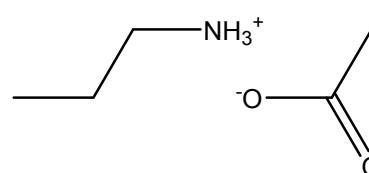
n-ethylammonium acetate

[N2A]



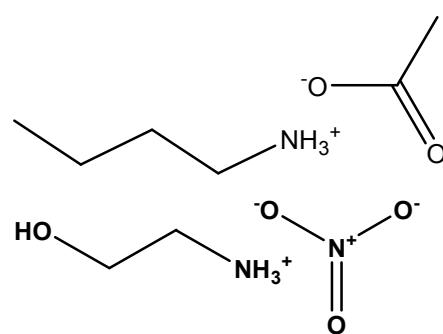
n-propylammonium acetate

[N3A]



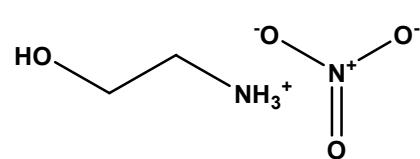
n-butylammonium acetate

[N4A]



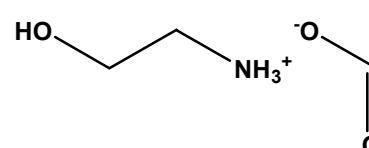
Ethanolammonium nitrate

[EOAN]



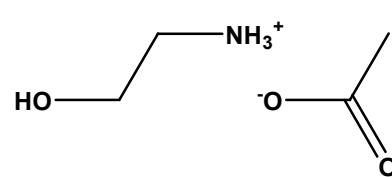
Ethanolammonium formate

[EOAF]



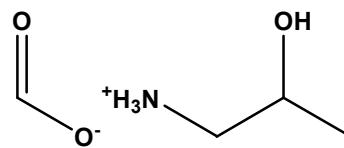
Ethanolammonium acetate

[EOAA]



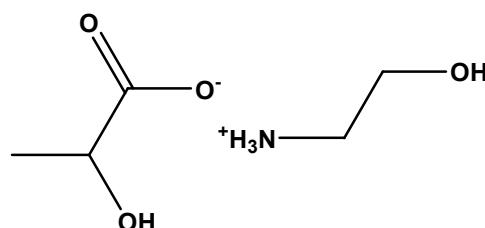
2-propanolammonium formate

[2-POAF]

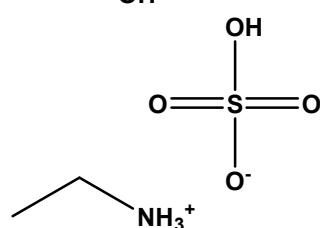


Ethanolammonium lactate

[EOAL]

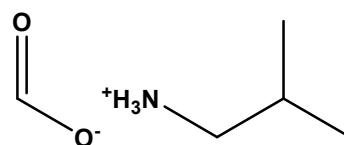


Ethylammonium hydrogen sulfate [EAHS]

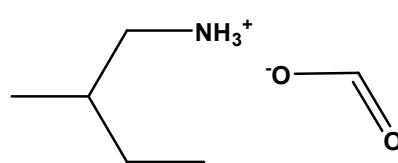


2-methylpropylammonium  
formate

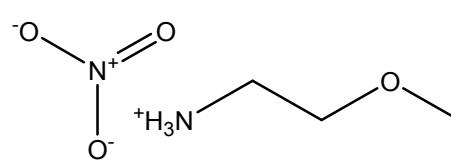
[2-MPAF]



2-methylbutylammonium formate [2-MBAF]

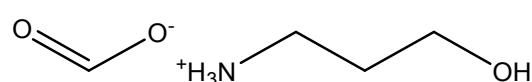


2-methoxyethylammonium nitrate [MEOEAN]



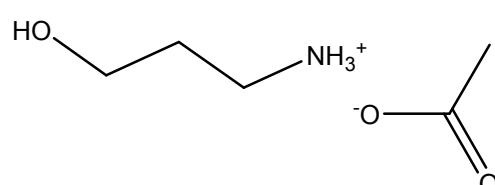
3-hydroxypropylammonium  
formate

[3-HPAF]



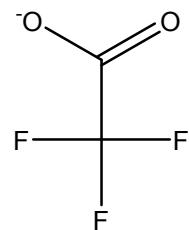
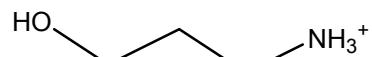
3-hydroxypropylammonium  
acetate

[3-HPAA]



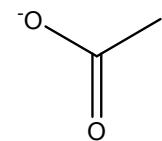
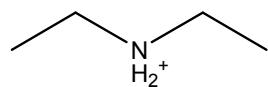
3-hydroxypropylammonium  
trifluoroacetate

[3-HPATFA]

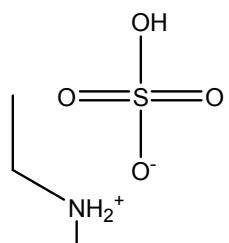


Diethylammonium acetate

[DEAA]

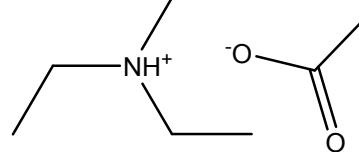


Diethyl ammonium hydrogen sulfate [DEAS]



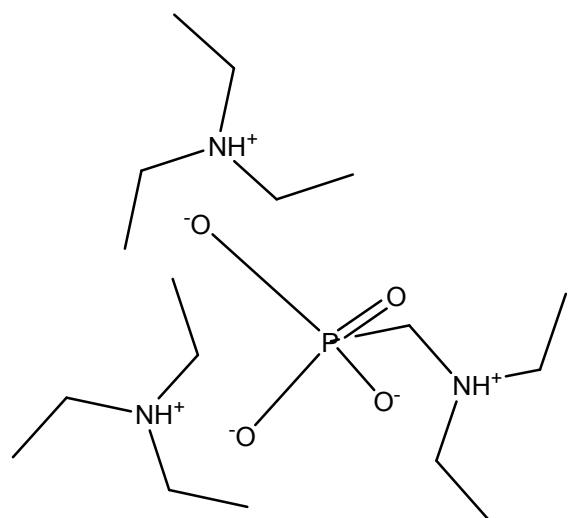
Triethylammonium acetate

[TEAA]

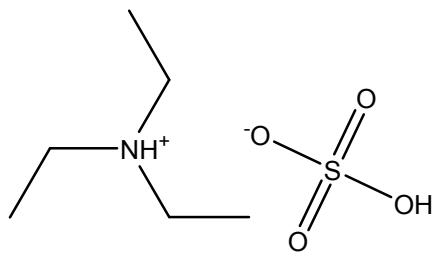


Triethylammonium phosphate

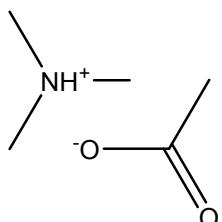
[TEAP]



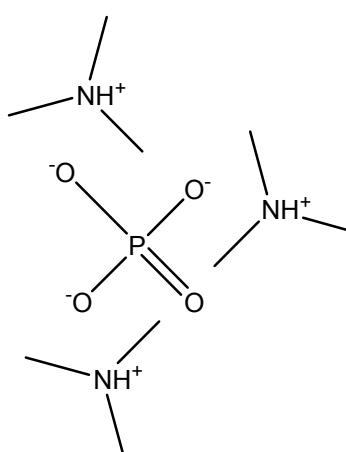
Triethylammonium      hydrogen [TEAS]  
sulfate



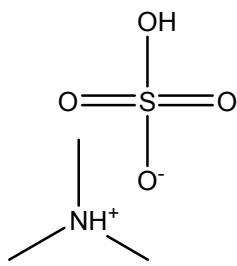
Trimethylammonium acetate      [TMAA]



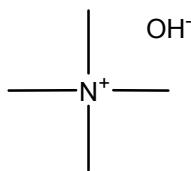
Trimethylammonium phosphate      [TMAP]



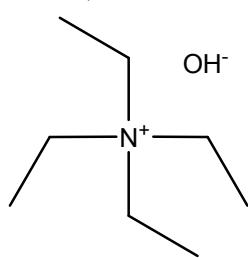
Trimethylammonium      hydrogen [TMAS]  
sulfate



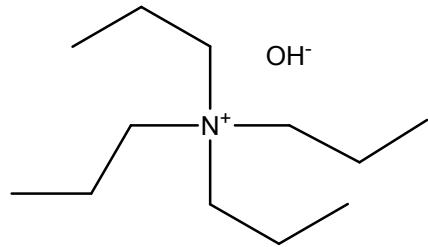
Tetramethylammonium hydroxide      [TMAH]



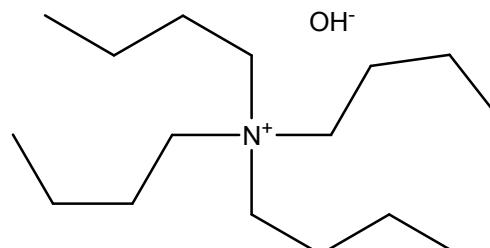
Tetraethylammonium hydroxide      [TEAH]



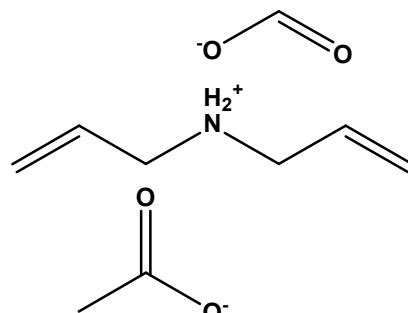
Tetrapropylammonium hydroxide [TPAH]



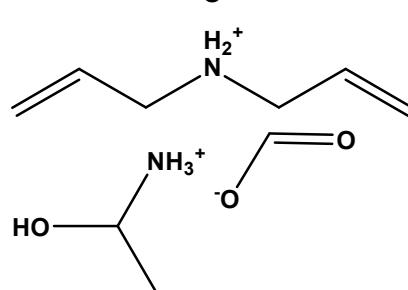
Tetrabutylammonium hydroxide [TBAH]



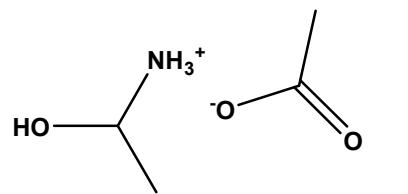
Diallylammonium formate [DAAF]



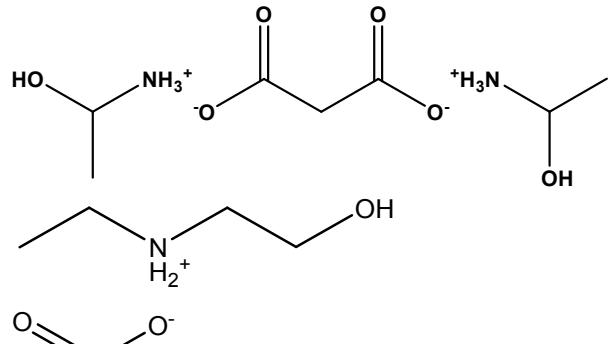
Diallylammonium acetate [DAAA]



1-hydroxyethylammonium formate [HEAF]

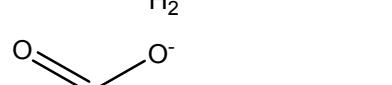


1-hydroxyethylammonium acetate [HEAA]



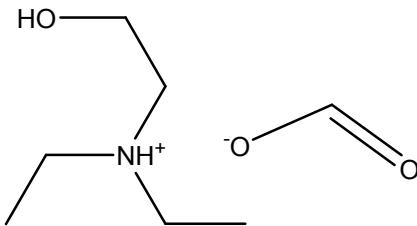
1-hydroxyethylammonium malonate [HEAMal]

2-hydroxydiethylammonium formate [2-HDEAF]

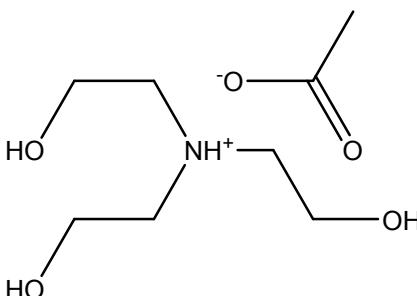


2-hydroxytriethylammonium  
formate

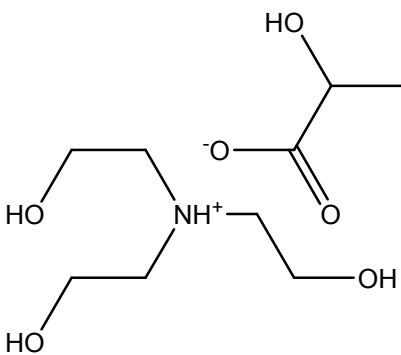
[2-HTEAF]



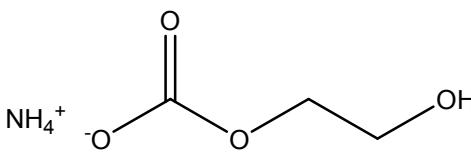
tri-(2-hydroxyethyl) ammonium [THEAA]  
acetate



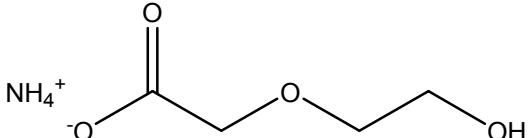
tri-(2-hydroxyethyl) ammonium [THEAL]  
lactate



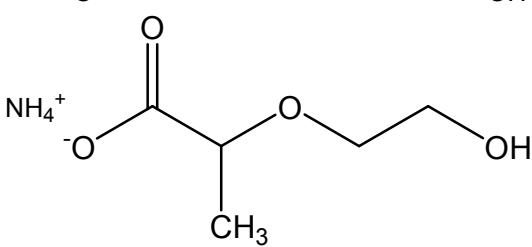
2-(2-hydroxyethoxy) ammonium [2,2-HEOAF]  
formate



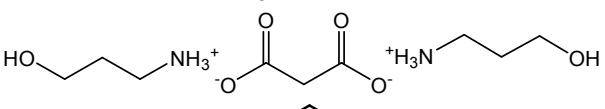
2-(2-hydroxyethoxy) ammonium [2,2-HEOAA]  
acetate



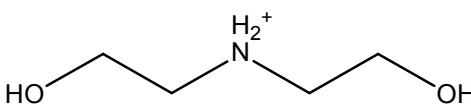
2-(2-hydroxyethoxy)ammonium [2,2-HEOAL]  
lactate



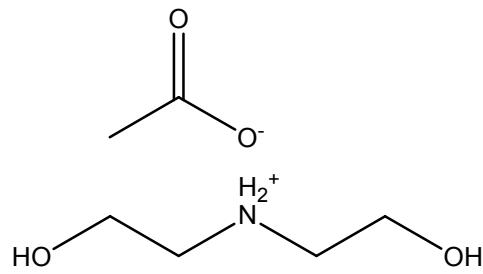
3-hydroxypropylammonium [3-HPAMal]  
malonate



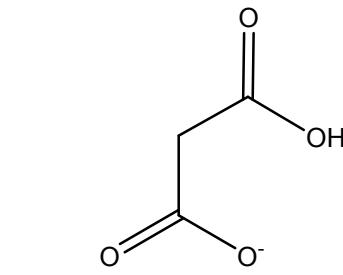
Bis(2-hydroxyethyl)ammonium [BHEAF]  
formate



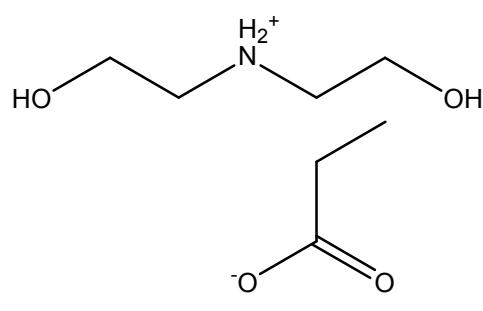
Bis(2-hydroxyethyl)ammonium [2-BHEAA]  
acetate



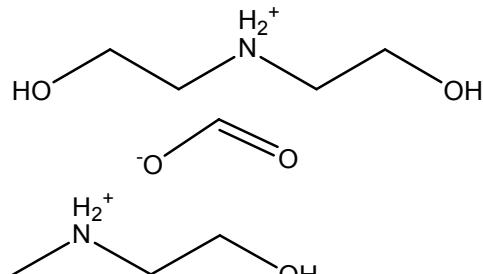
Bis(2-hydroxyethyl) ammonium [DEAMal]  
malonate



Bis(2-hydroxyethyl)ammonium [2-BHEAP]  
propionate

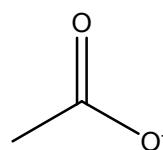


N-Methyl-2-hydroxyethyl  
ammonium formate



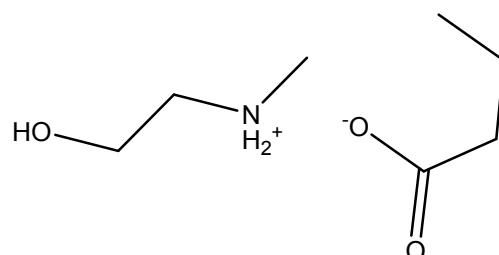
N-Methyl-2-  
hydroxyethylammonium acetate

[m-2-HEAA]



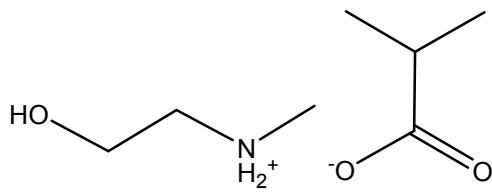
N-methyl-2-  
hydroxyethylammonium butyrate

[m-2-HEAB]



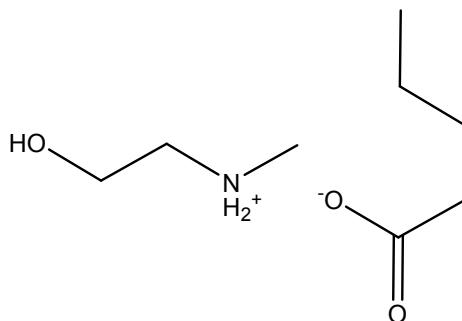
N-Methyl-2-hydroxyethylammonium isobutyrate

[m-2-HEAiB]



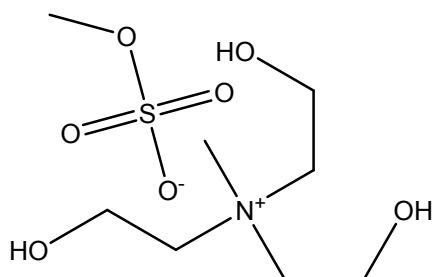
N-Methyl-2-hydroxyethylammonium pentanoate

[m-2-HEAP]



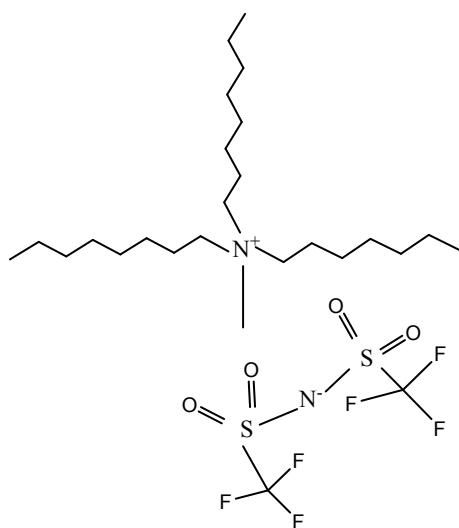
Tris(2-hydroxyethyl)methyl ammonium methylsulfate

[MTEOA][MeOSO<sub>3</sub>]



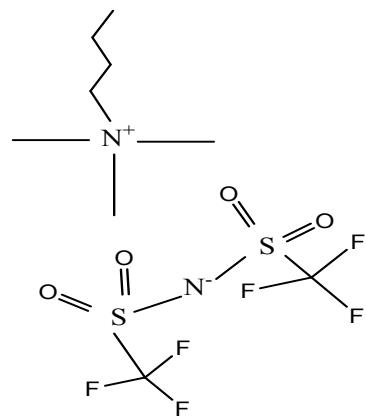
Methyltriocylammonium bis(trifluoromethylsulfonyl) imide

[MOA]<sup>+</sup>[Tf<sub>2</sub>N]<sup>-</sup>



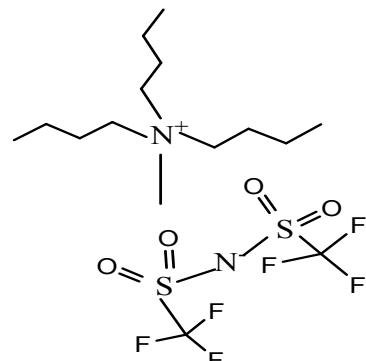
Trimethylbutylammonium  
bis(trifluoromethylsulfonyl) imide

[N<sub>1114</sub>][Tf<sub>2</sub>N]



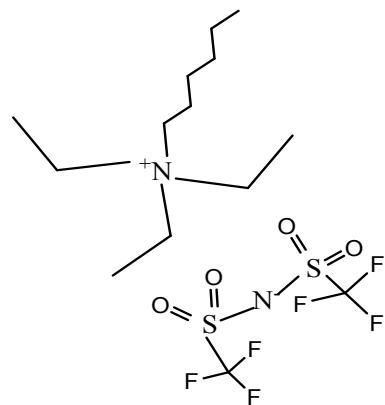
Tributylmethylammonium  
bis(trifluoromethylsulfonyl) imide

[N<sub>4441</sub>][Tf<sub>2</sub>N]



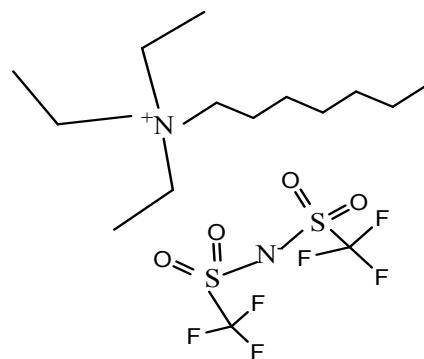
N-hexyl-triethylammonium  
bis(trifluoromethylsulfonyl)imide

[N<sub>6,222</sub>][Tf<sub>2</sub>N]

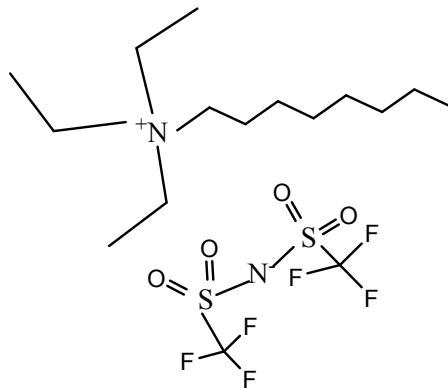
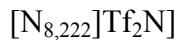


N-heptyl-triethylammonium  
bis(trifluoromethylsulfonyl)imide

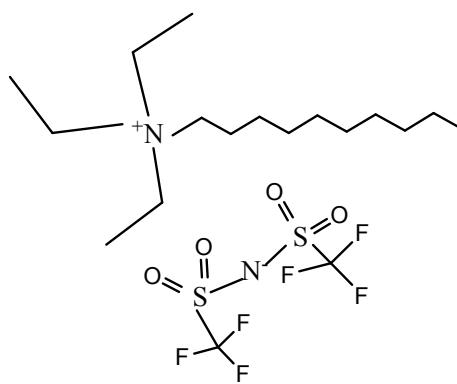
[N<sub>7,222</sub>][Tf<sub>2</sub>N]



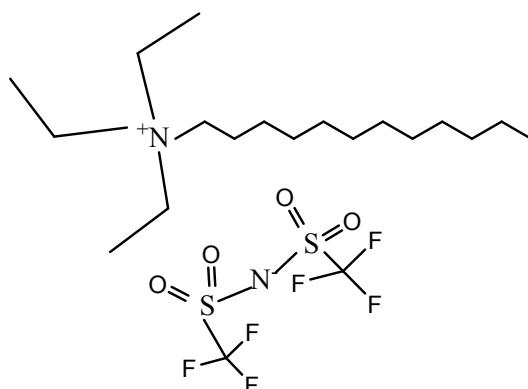
## N-octyl-triethylammonium bis(trifluoromethylsulfonyl)imide



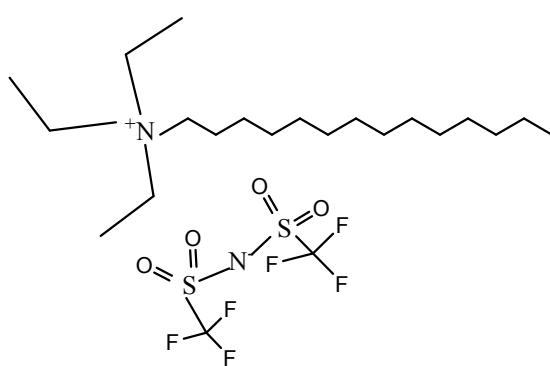
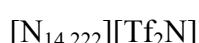
## N-docyl-triethylammonium bis(trifluoromethylsulfonyl)imide



## N-dodecyl-triethylammonium bis(trifluoromethylsulfonyl)imide

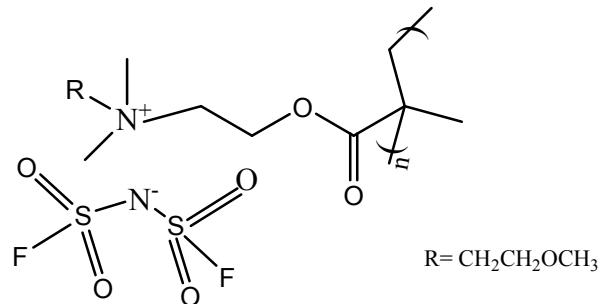


## N-tetradecyl-triethylammonium bis(trifluoromethylsulfonyl)imide



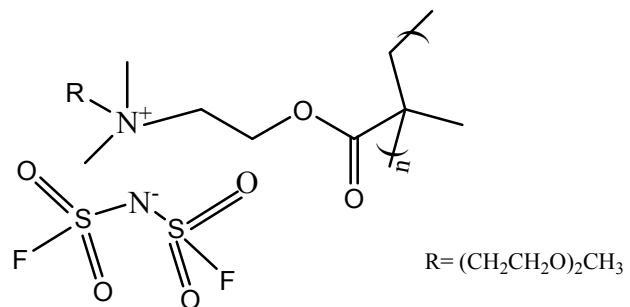
Poly(N,N-dimethyl-N-[2-(methacryloyloxy)ethyl]-N-(2-methoxyethyl)ammonium) bis(fluorosulfonyl)imide

( $[C_3ON_{MA,11}]FSI$ )



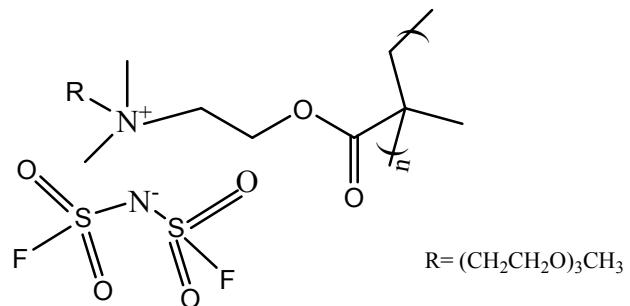
Poly(N,N-dimethyl-N-[2-(methacryloyloxy)ethyl]-N-(2-methoxyethyl)ammonium) bis(fluorosulfonyl)imide

( $[C_5O_2N_{MA,11}]FSI$ )



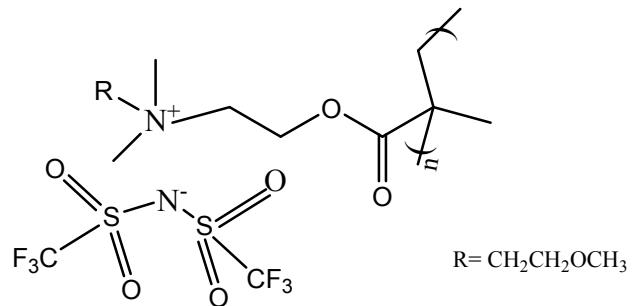
Poly(N,N-dimethyl-N-[2-(methacryloyloxy)ethyl]-N-[2-(2-methoxyethoxy)ethyl]ammonium) bis(fluorosulfonyl)imide

( $[C_7O_3N_{MA,11}]FSI$ )



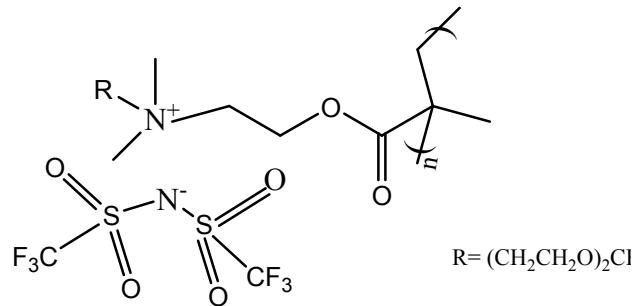
Poly(N,N-dimethyl-N-[2-(methacryloyloxy)ethyl]-N-(2-methoxyethyl)ammonium) bis(trifluorosulfonyl)imide

( $[C_3ON_{MA,11}]TFSI$ )



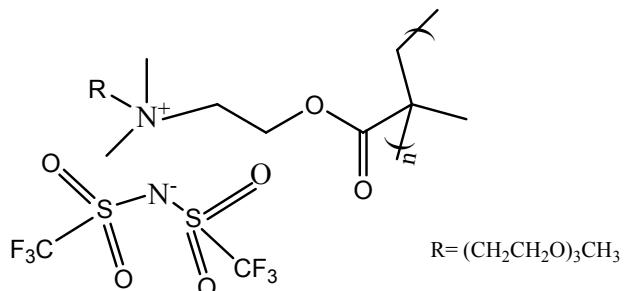
Poly(N,N-dimethyl-N-[2-(methacryloyloxy)ethyl]-N-[2-(2-methoxyethyl)ammonium) bis(trifluorosulfonyl)imide

( $[C_5O_2N_{MA,11}]TFSI$ )



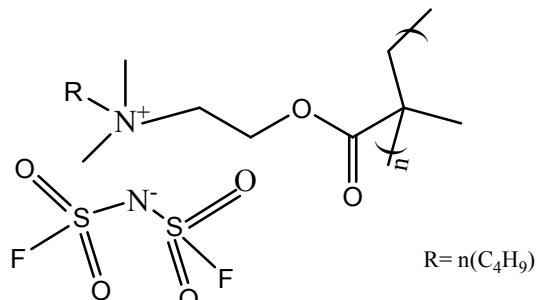
Poly(N,N-dimethyl-N-[2-(methacryloyloxy)ethyl]-N-[2-(2-methoxyethoxy)ethyl]ammonium)  
bis(trifluorosulfonyl)imide

( $[C_7O_3N_{MA,11}]TFSI$ )



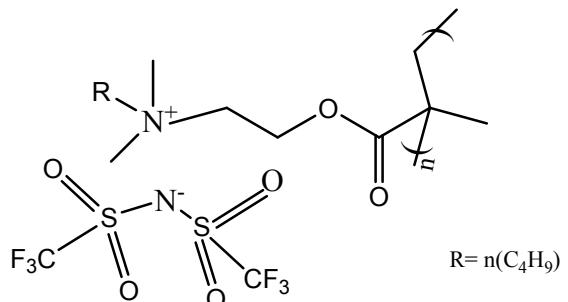
Poly(N-(n-butyl)-N,N-dimethyl-N-[2-(methacryloyloxy)ethyl]ammonium)  
bis(fluorosulfonyl)imide

( $[C_4N_{MA,11}]FSI$ )



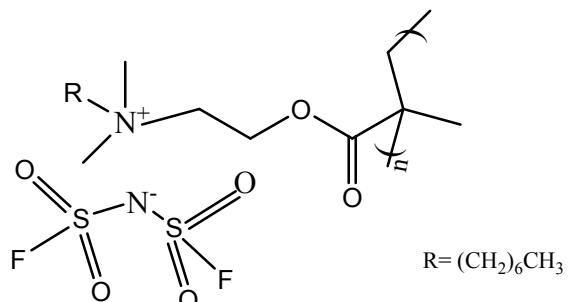
Poly(N-(n-butyl)-N,N-dimethyl-N-[2-(methacryloyloxy)ethyl]ammonium)  
bis(trifluoromethanesulfonyl)imid

( $[C_4N_{MA,11}]TFSI$ )



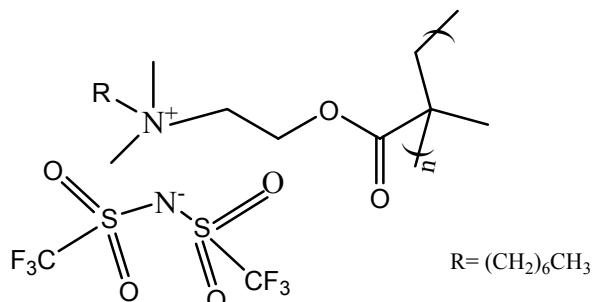
Poly(N,N-dimethyl-N-(n-butyl)-N-[2-(methacryloyloxy)ethyl]-N-(2-methoxyethyl)ammonium)  
bis(fluorosulfonyl)imide

( $[C_7N_{MA,11}]FSI$ )



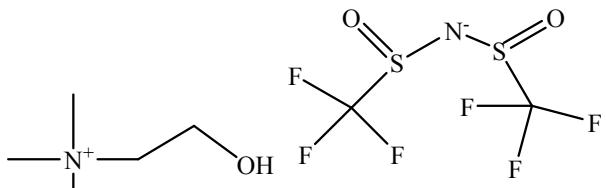
Poly(N,N-dimethyl-N-(n-heptyl)-N-[2-(methacryloyloxy)ethyl]-N-(2-methoxyethyl)ammonium)  
bis(trifluorosulfonyl)imide

( $[C_7N_{MA,11}]TFSI$ )



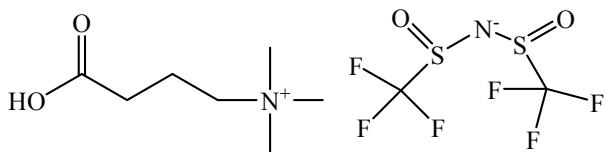
(2-hydroxyethyl)trimethyl ammoniumbis(trifluoro-methylsulfonyl)imide

[N<sub>1112OH</sub>][NTf<sub>2</sub>]



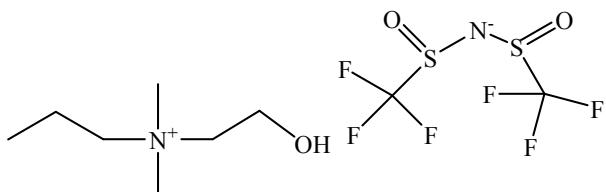
N,N,N-trimethylammonium - N-butanoic acid bis[(trifluoromethylsulfonyl)imid

[N<sub>4COOH111</sub>][Tf<sub>2</sub>N]



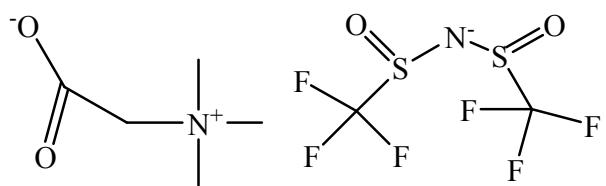
(2-hydroxyethyl) dimethylpropylammonium bis(trifluoro-methylsulfonyl) imide

[N<sub>1132OH</sub>][Tf<sub>2</sub>N]



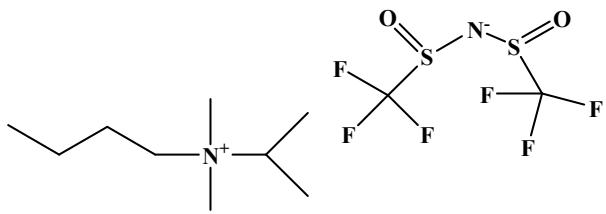
(2-acetate)trimethylammonium bis(trifluoro-methylsulfonyl) imide

[N<sub>1112OOCCH3</sub>][Tf<sub>2</sub>N]



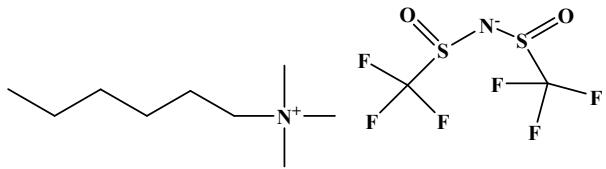
dimethyl(butyl(i-propyl)) ammonium bis-(trifluoromethylsulfonyl)imide

[N(4)113][Tf<sub>2</sub>N]



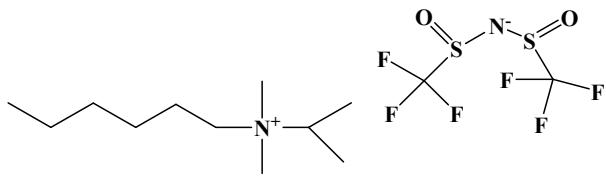
trimethyl-(hexyl) ammonium bis(trifluoromethylsulfonyl)imide

[N(6)111][Tf<sub>2</sub>N]



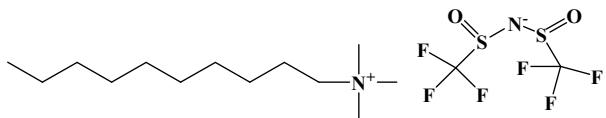
dimethyl-(hexyl)(i-propyl) bis(trifluoromethylsulfonyl)imide

[N(6)113][Tf<sub>2</sub>N]



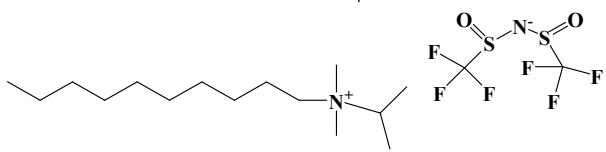
trimethyl(decyl)ammonium bis(trifluoromethylsulfonyl) imide

[N(10)111][Tf<sub>2</sub>N]



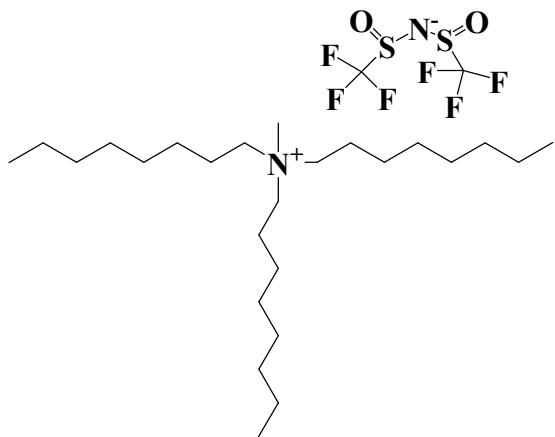
dimethyl(decyl(i-propyl)) bis(trifluoromethylsulfonyl)imide

[N(10)113][Tf<sub>2</sub>N]



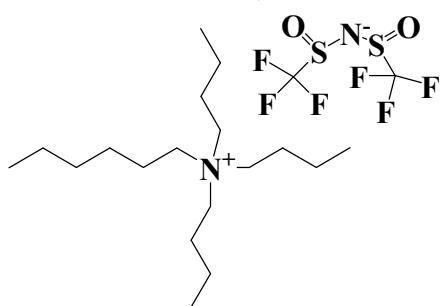
trioctyl(methyl)ammonium  
bis(trifluoromethylsulfonyl) imide

[N(1)888][Tf<sub>2</sub>N]



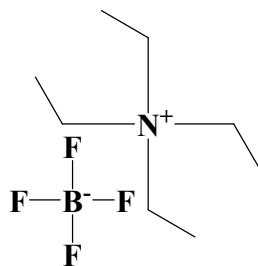
tributylhexylammonium  
bis(trifluoromethylsulfonyl)imide

[N<sub>4,4,4,6</sub>][NTf<sub>2</sub>]



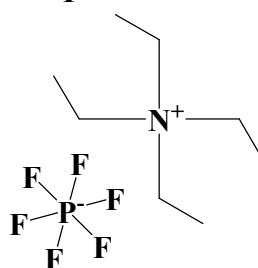
N,N,N,N-tetraethyl  
ammoniumtetrafluoroborate

[N<sub>2222</sub>]BF<sub>4</sub>



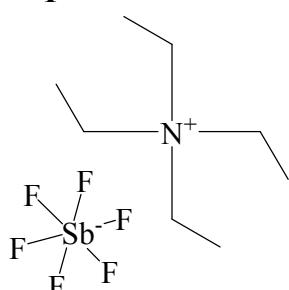
N,N,N,N-tetraethyl  
ammoniumhexafluorophosphate

[N<sub>2222</sub>]PF<sub>6</sub>



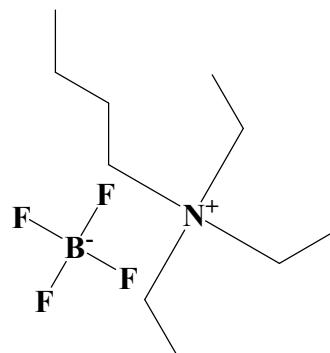
N,N,N,N-tetraethyl  
ammoniumhexafluoroantimonate

[N<sub>2222</sub>]SbF<sub>6</sub>



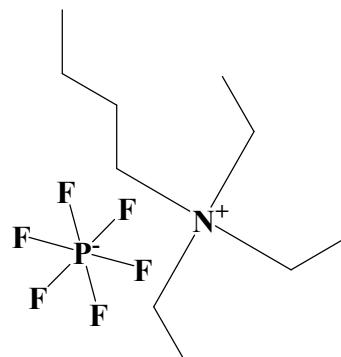
N,N,N-triethylbutyl  
ammoniumtetrafluoroborate

[N<sub>2224</sub>]BF<sub>4</sub>



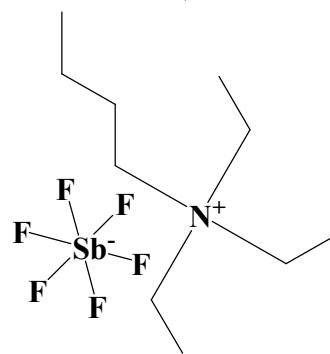
N,N,N-triethylbutyl  
ammoniumhexafluorophosphate

[N<sub>2224</sub>]PF<sub>6</sub>



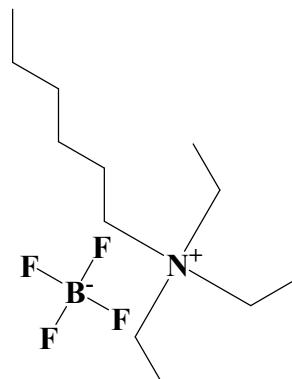
N,N,N-triethylbutyl  
ammoniumhexafluoroantimonate

[N<sub>2224</sub>]SbF<sub>6</sub>



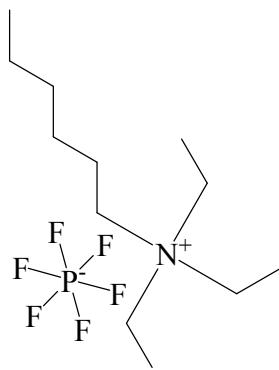
N,N,N-triethylhexyl  
ammoniumtetrafluoroborate

[N<sub>2226</sub>]BF<sub>4</sub>



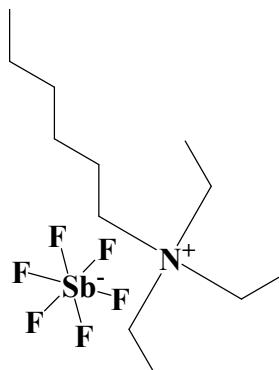
N,N,N-triethylhexyl  
ammoniumhexafluorophosphate

[N<sub>2226</sub>]PF<sub>6</sub>



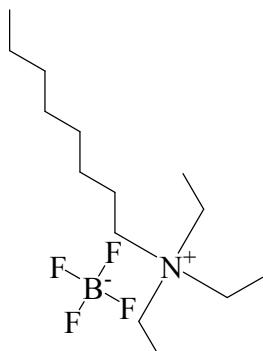
N,N,N-triethylhexyl  
ammoniumhexafluoroantimonate

[N<sub>2226</sub>]SbF<sub>6</sub>



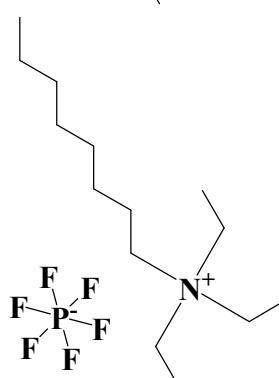
N,N,N-triethyloctyl  
ammoniumtetrafluoroborate

[N<sub>2228</sub>]BF<sub>4</sub>



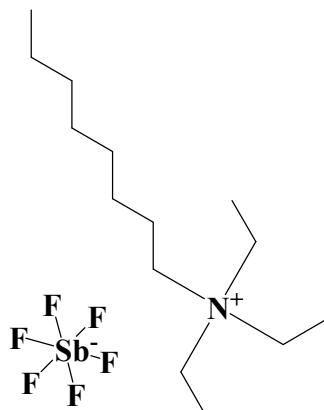
N,N,N-triethyloctyl  
ammoniumhexafluorophosphate

[N<sub>2228</sub>]PF<sub>6</sub>



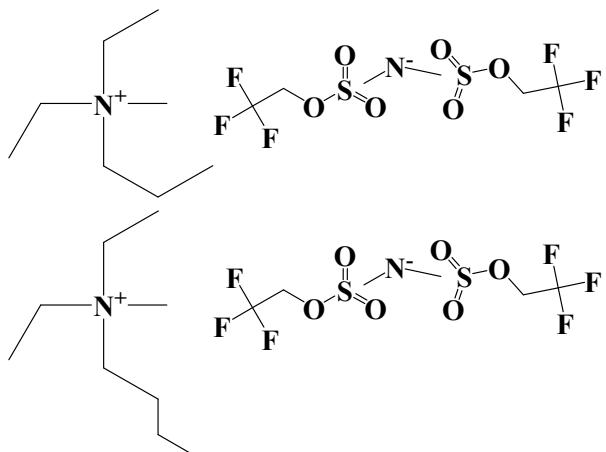
N,N,N-triethyloctyl  
ammoniumhexafluoroantimonate

[N<sub>2228</sub>]SbF<sub>6</sub>



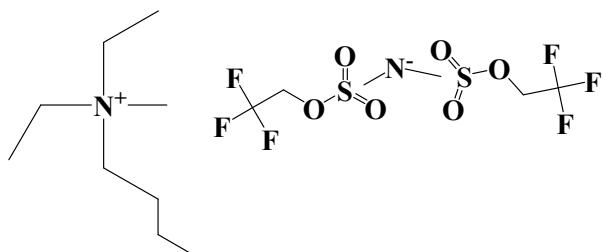
N,N-Diethyl-N-methyl-N-(n-propyl)ammonium bis (2,2,2-trifluoroethoxy sulfonyl)imide

(N<sub>1223</sub>[TFESI])



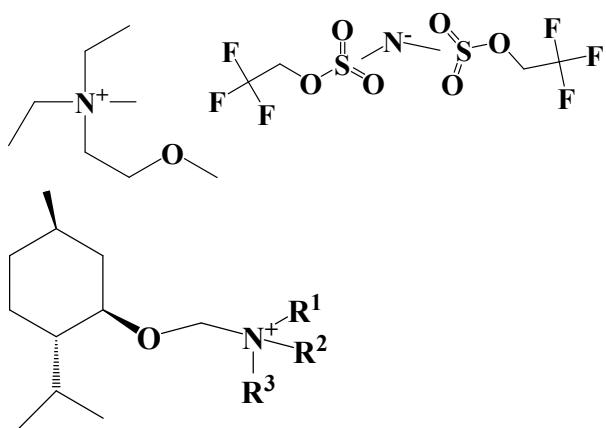
N-(n-Butyl)-N,N-diethyl-N-methylammonium  
bis(2,2,2-trifluoroethoxy sulfonyl)imide

(N<sub>1224</sub>[TFESI])



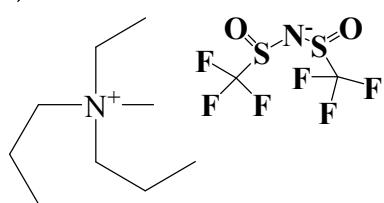
N,N-Diethyl-N-methyl-N-(2-methoxyethyl) ammonium  
bis(2,2,2-trifluoroethoxysulfonyl)  
imide

(N<sub>122.1O2</sub>[TFESI])



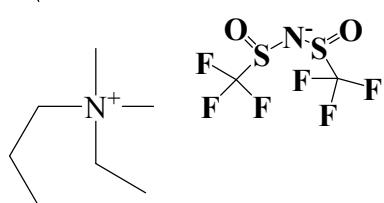
Trialkyl[(1R,2S,5R)-(-)-  
mentoxymethyl] ammonium  
bis(trifluoromethanesulfonyl)imid  
es

[N<sub>1233</sub>][TFSI]



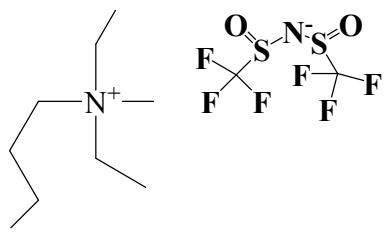
methylethyldipropyl ammonium  
bis(trifluorosulfonyl)imide

[N<sub>1123</sub>][TFSI]



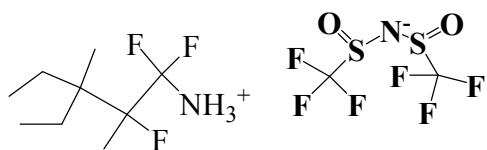
diethylmethylbutyl ammonium  
bis(trifluorosulfonyl)imide

[N<sub>1224</sub>][TFSI]



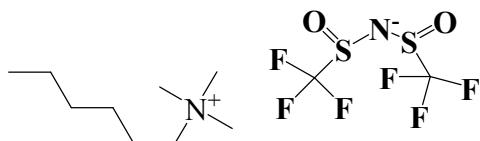
diethylmethyltrifluorobutyl  
ammonium bis(trifluorosulfonyl)  
imide

[N<sub>1224f</sub>][TFSI]



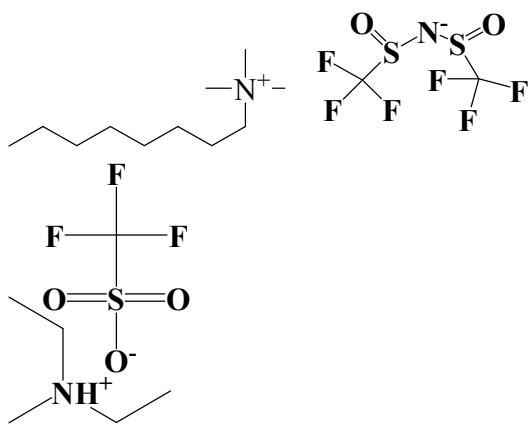
trimethylhexylammonium  
bis(trifluorosulfonyl)imide

[N<sub>1116</sub>][TFSI]



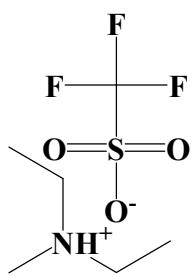
trimethyloctylammonium  
bis(trifluorosulfonyl)imide

[N<sub>1118</sub>][TFSI]



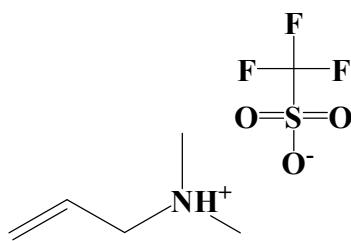
diethylmethylammonium  
trifluoromethanesulfonate

([N122][TfO])



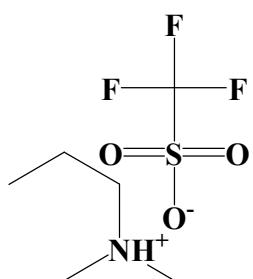
allyldimethylammonium  
trifluoromethanesulfonate

([N11a][TfO])



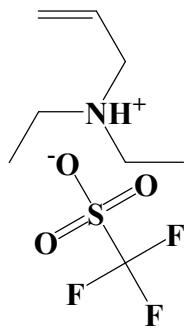
dimethylpropylammonium  
trifluoromethanesulfonate

[N113][TfO]



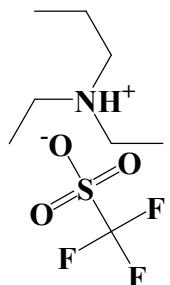
allyldiethylammonium  
trifluoromethanesulfonate

[N22a][TfO]



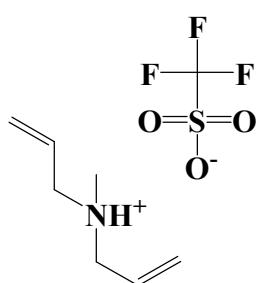
diethylpropylammonium  
trifluoromethanesulfonate

[N223][TfO]



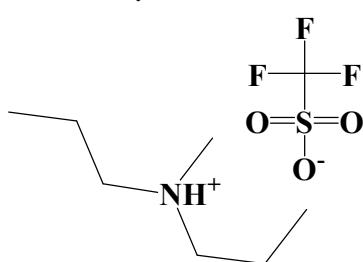
diallylmethylammonium  
trifluoromethanesulfonate

[N1aa][TfO]



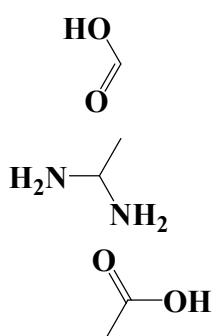
dipropylmethylammonium  
trifluoromethanesulfonate

[N133][TfO]



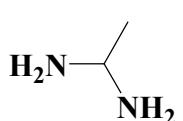
Ethanediamine formic acid

[EDA.HO<sub>2</sub>CH]



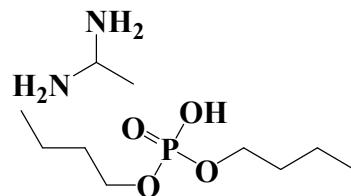
Ethanediamine acetic acid

[EDA.AcOH]



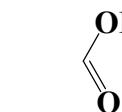
Ethanediamine di-n-butyl phosphate

[EDA.(BuO)<sub>2</sub>PO<sub>2</sub>H]



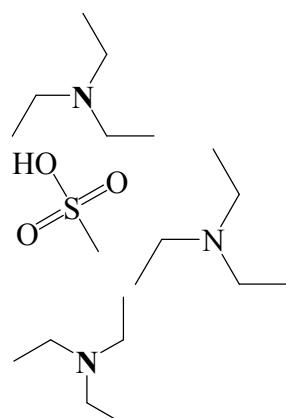
Triethylamine formic acid

[Et<sub>3</sub>N.HO<sub>2</sub>CH]



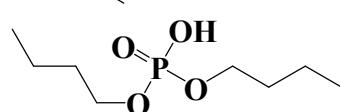
Triethylamine methylsulfonic acid

[Et<sub>3</sub>N.MsOH]



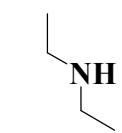
Triethylamine di-n-butyl phosphate

[Et<sub>3</sub>NH.(BuO)<sub>2</sub>PO<sub>2</sub>H]



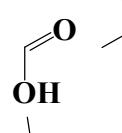
Diethylamine di-n-butyl phosphate

[Et<sub>2</sub>NH.(BuO)<sub>2</sub>PO<sub>2</sub>H]



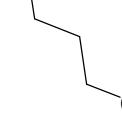
Di-n-Butylamine formic acid

[Bu<sub>2</sub>NH.HO<sub>2</sub>CH]



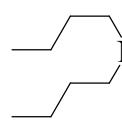
Tri-n-Butylamine di-n-butyl phosphate

Bu<sub>3</sub>N.(BuO)<sub>2</sub>PO<sub>2</sub>H



diethanolamine formic acid

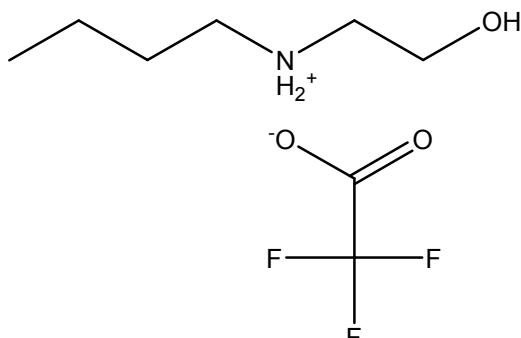
(HOEt)<sub>2</sub>N.HO<sub>2</sub>CH



diethanolamine acetic acid	$(HOEt)_2NH \cdot AcOH$	
diethanolamine sulfamic acid	$(HOEt)_2 NH \cdot OSA$	
diethanolamine methylsulfonic acid	$(HOEt)_2NH \cdot MsOH$	
diethanolamine di-n-butyl phosphate	$(HOEt)_2NH \cdot (BuO)_2P O_2H$	
diethanolamine Chlorid	[DEA][Cl]	
triethanolamine formate	[TEtA][Of]	
triethanolamine acetate	[TEtA][A]	
di-n-propylamine formate	[DPA][Of]	
Methyldiethanolamine	[MDEA]	

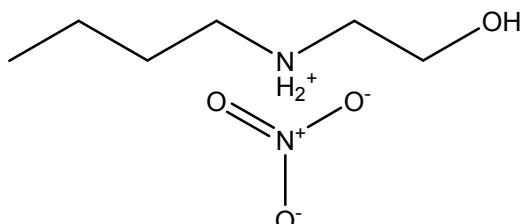
N-butyl-(N-hydroxyethyl)  
ammonium trifluoroacetate

[BHEA] [TFA]



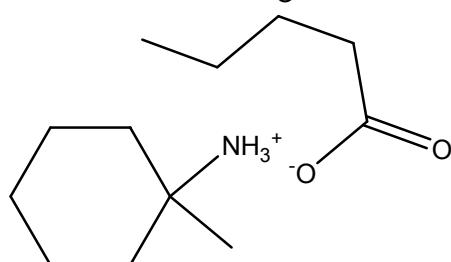
N-butyl-(N-hydroxyethyl)  
ammonium nitrate

[BHEA] [NO<sub>3</sub>]



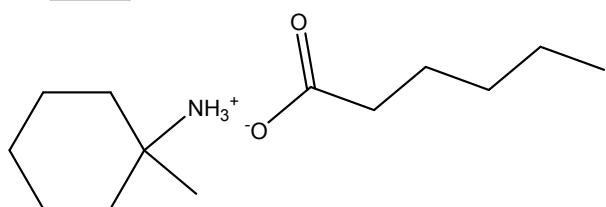
N-methylcyclohexyl ammonium  
pentanoate

[NMC][Pen]



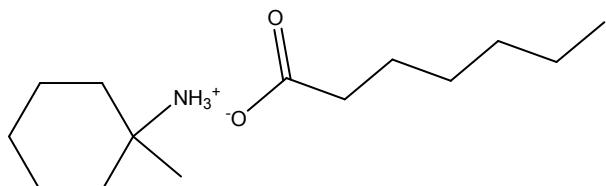
N-methylcyclohexyl ammonium  
hexanoate

[NMC][Hex]



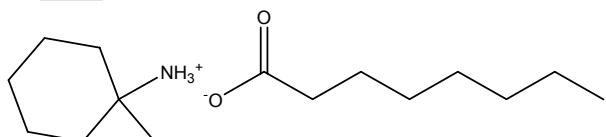
N-methylcyclohexyl ammonium  
heptanoate

[NMC][Hep]



N-methylcyclohexyl ammonium  
octanoate

[NMC][Oct]



N-ethyl-N,N-dimethyl  
ammoniumphenylacetate

[N<sub>112H</sub>][C<sub>7</sub>H<sub>7</sub>CO<sub>2</sub>]

