Stability of the Zwitterionic Liquid Butyl-Methyl-Imidazol-2-ylidene Borane

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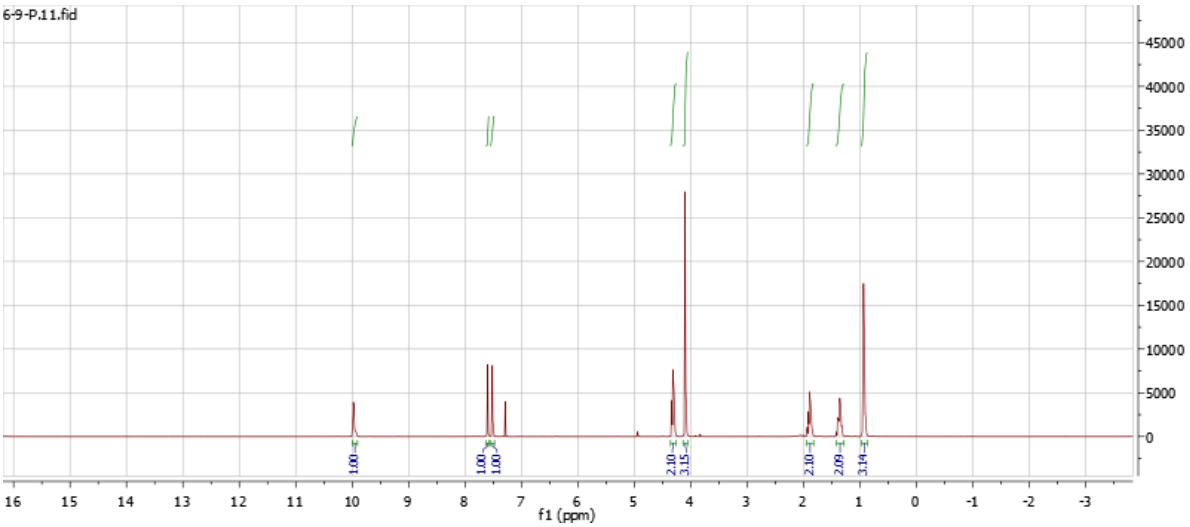
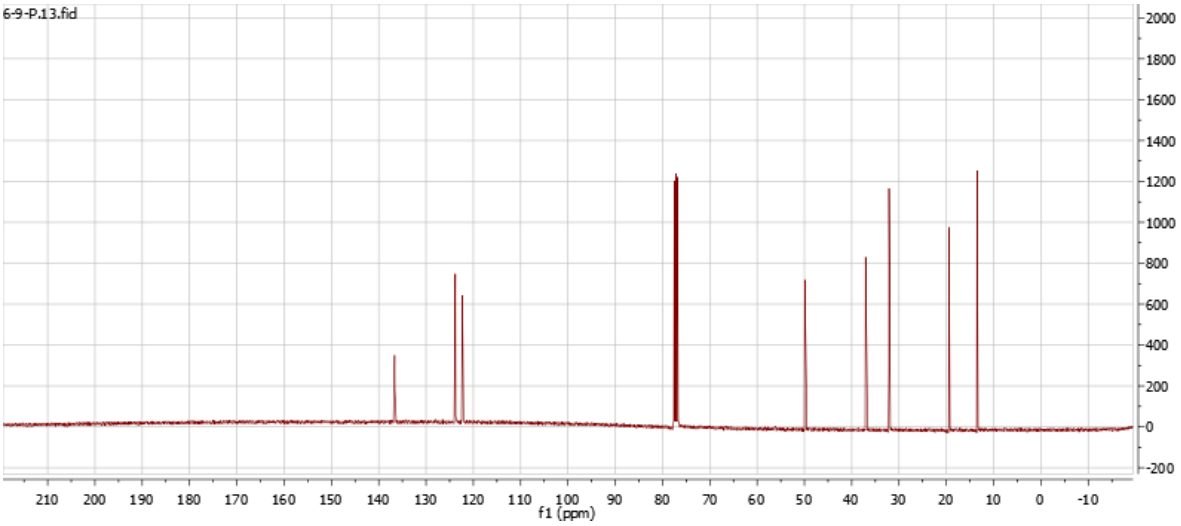
Supporting Information

Contents

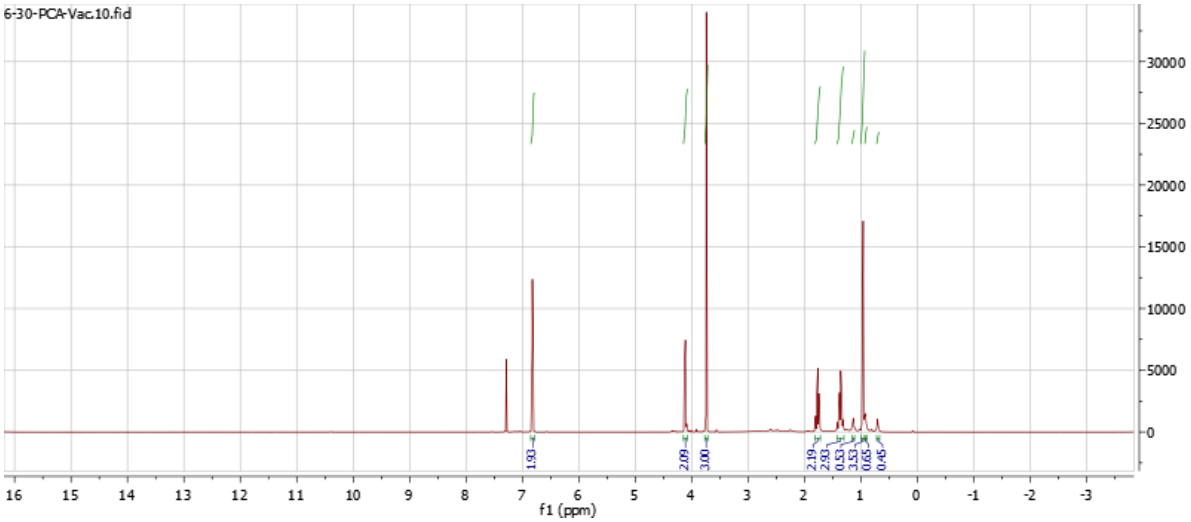
NMR-Spectra

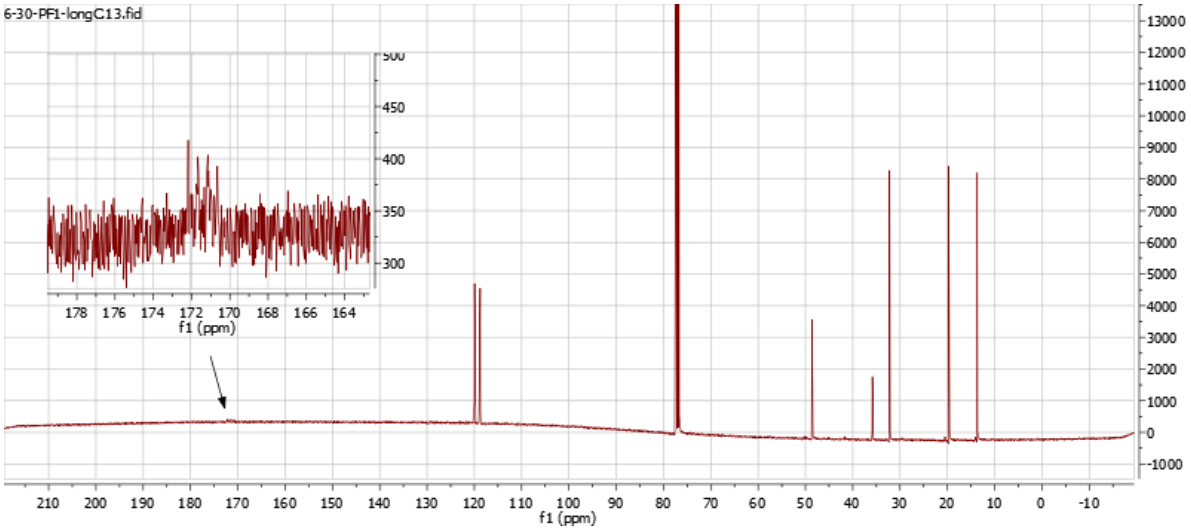
1-Butyl-3-methylimidazolium iodide (IL-H-I)



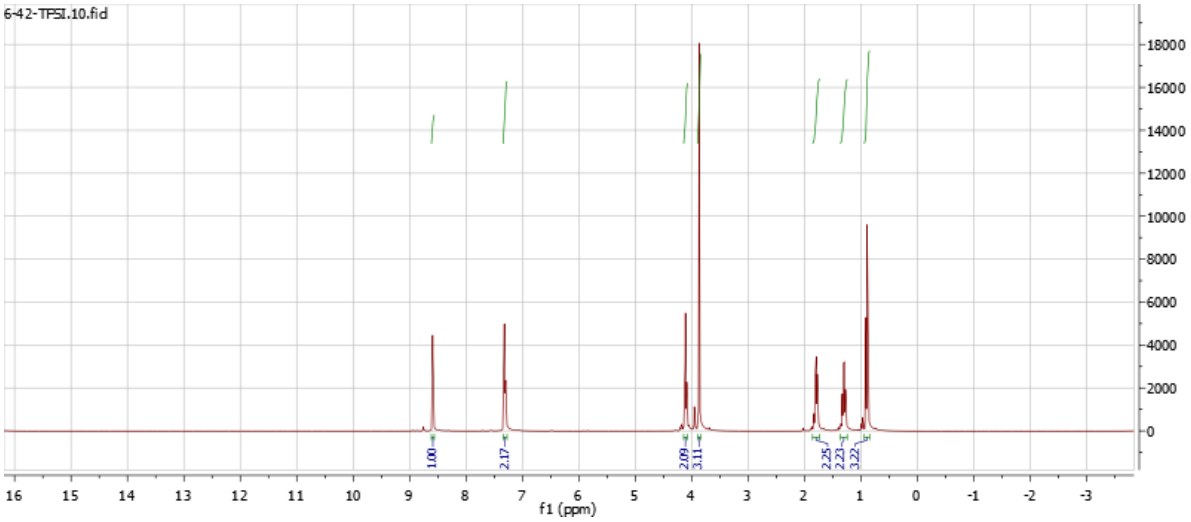


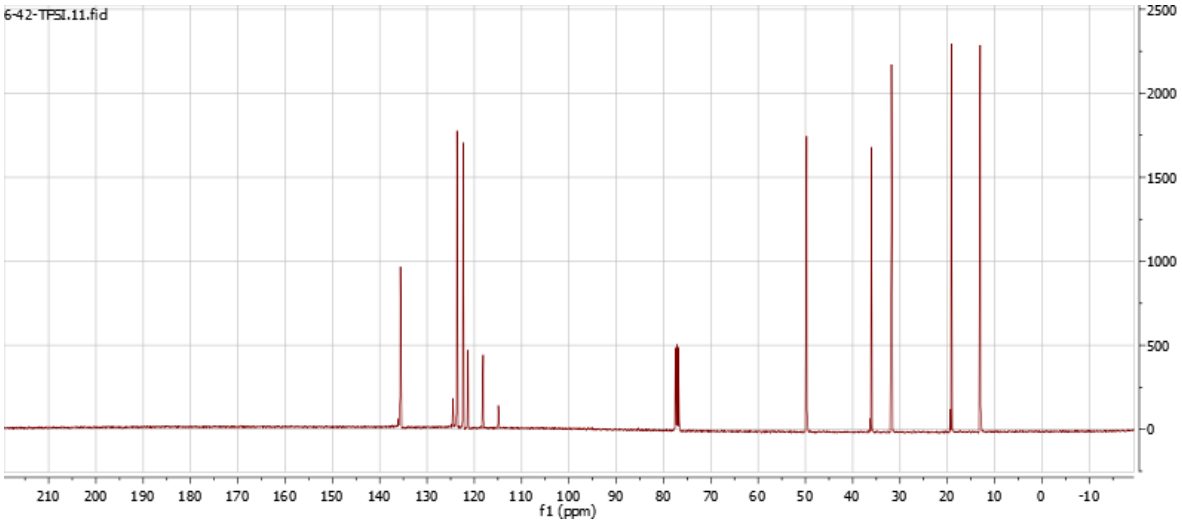
1-Butyl-3-methylimidazol-2-ylidene borane (ZIL)



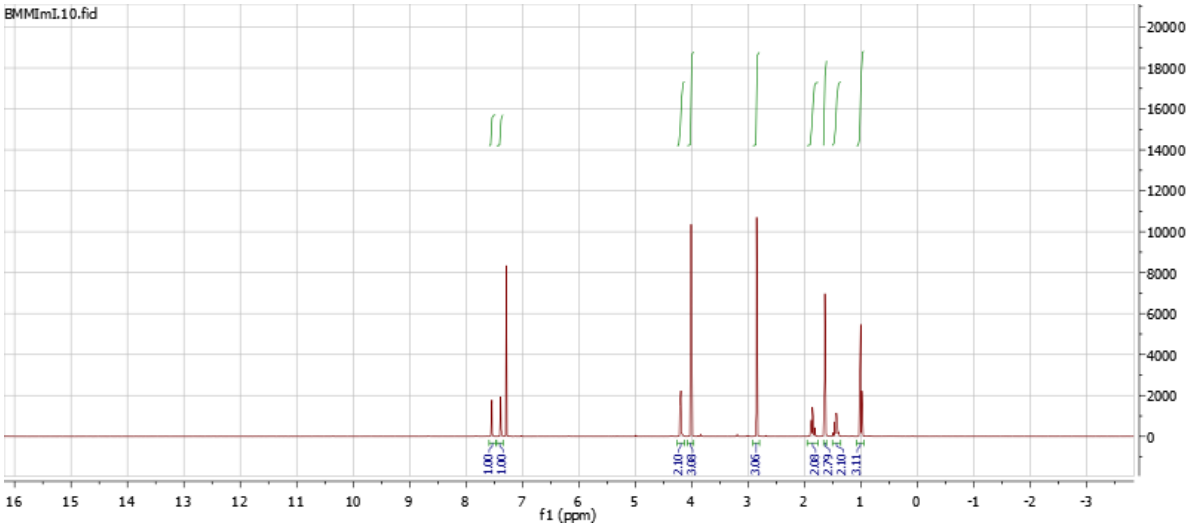


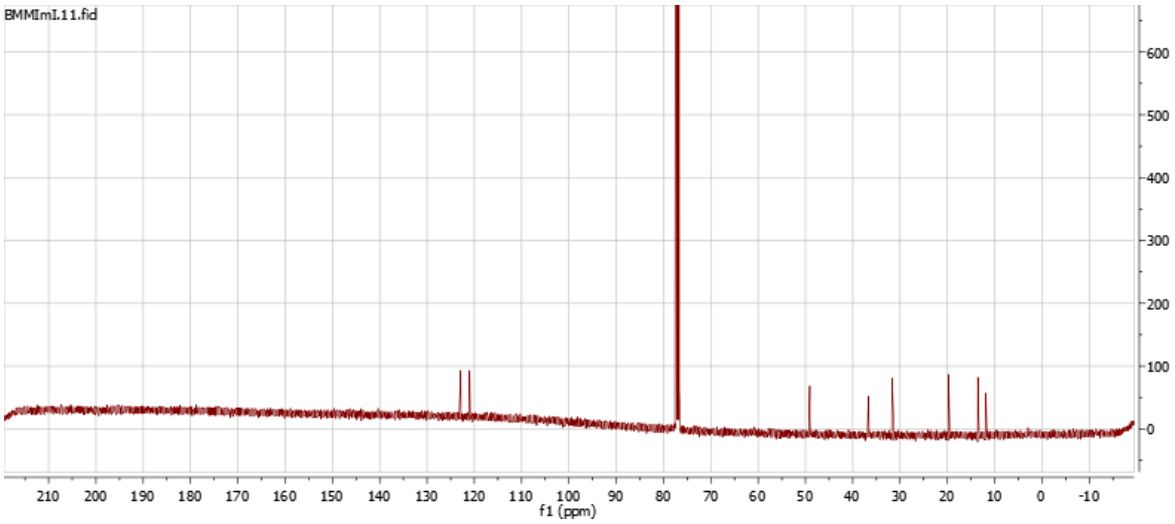
1-Butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide (IL-H-TFSI)



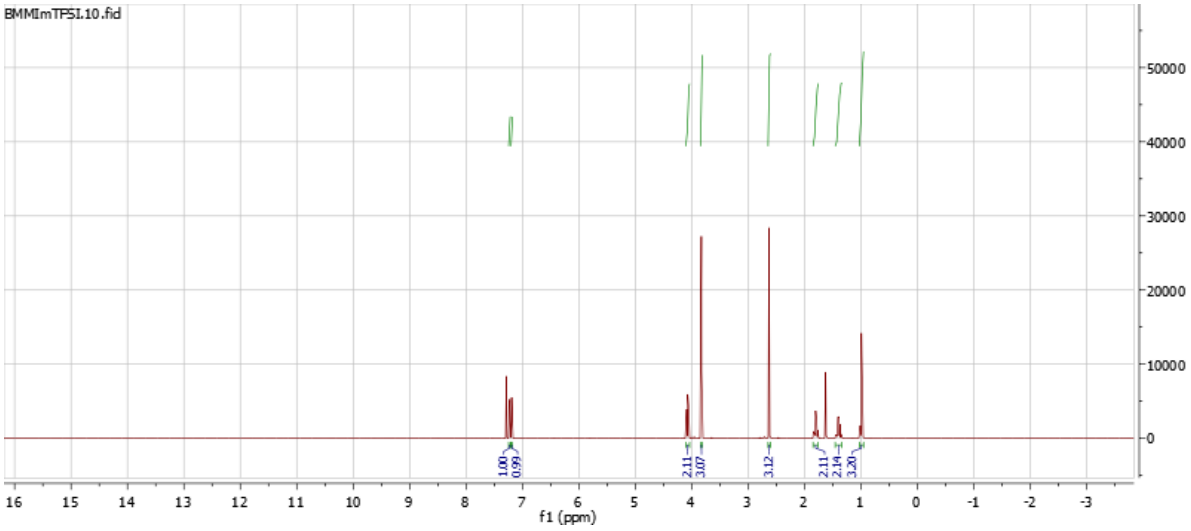


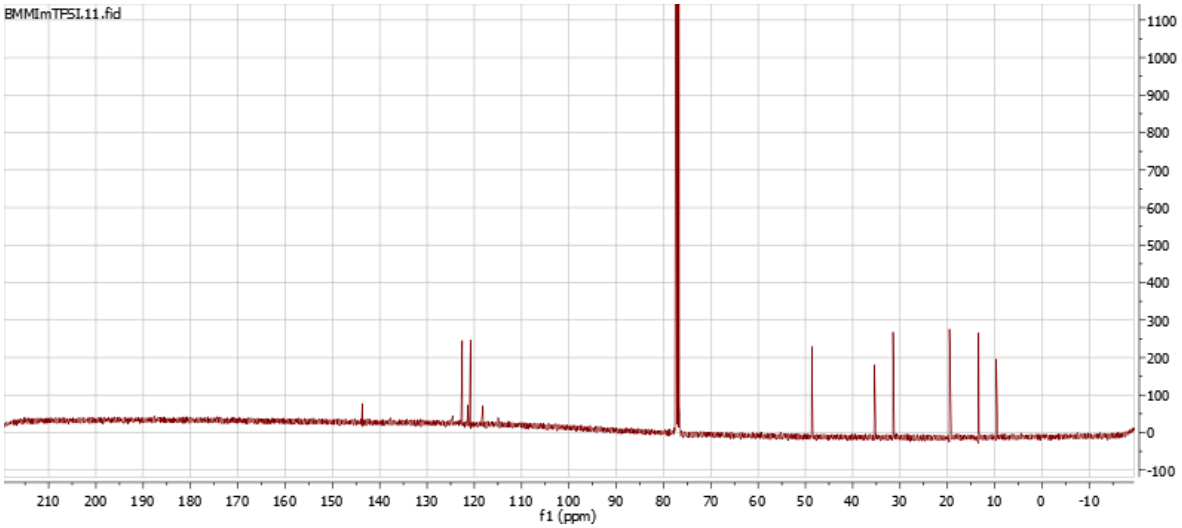
1-Butyl-2,3-dimethylimidazolium iodide (IL-Me-I)





1-Butyl-2,3-dimethylimidazolium bis(trifluoromethanesulfonyl)imide (IL-Me-TFSI)

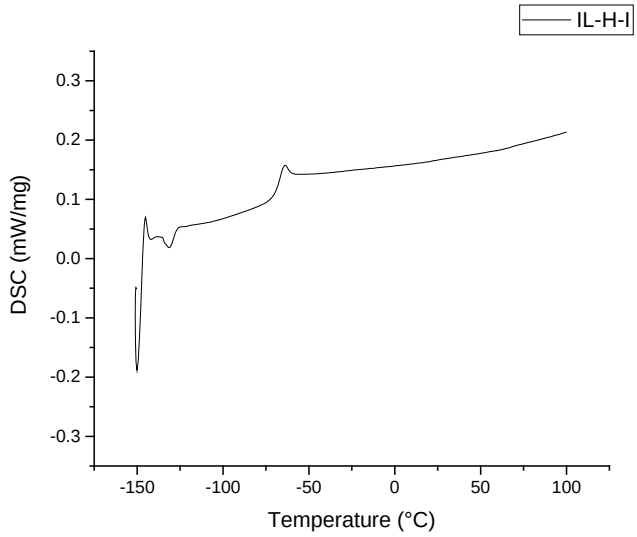




Differential Scanning Calorimetry

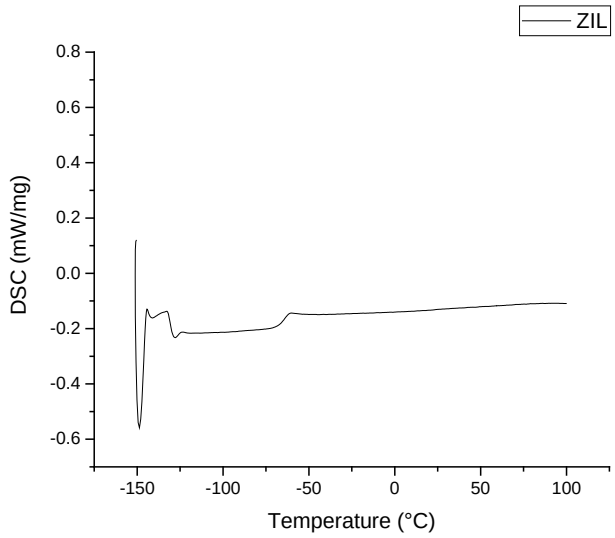
Graphs display the third heating phase. The irregular behavior below -120 °C results from instrumentalization.

1-Butyl-2-methylimidazolium iodide (IL-H-I)



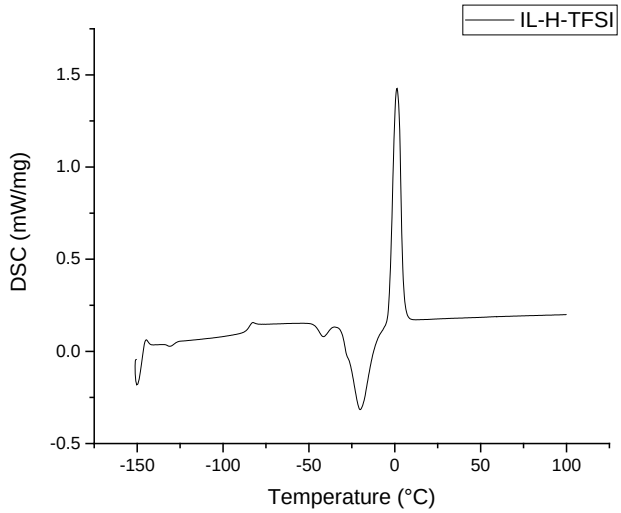
Glass transition: -68.3 °C, 0.243 J g^{-1} K^{-1}

1-Butyl-3-methylimidazol-2-ylidene borane (ZIL)



Glass transition: -64,9 °C, 0.305 J g^{-1} K^{-1}

1-Butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide (IL-H-TFSI)

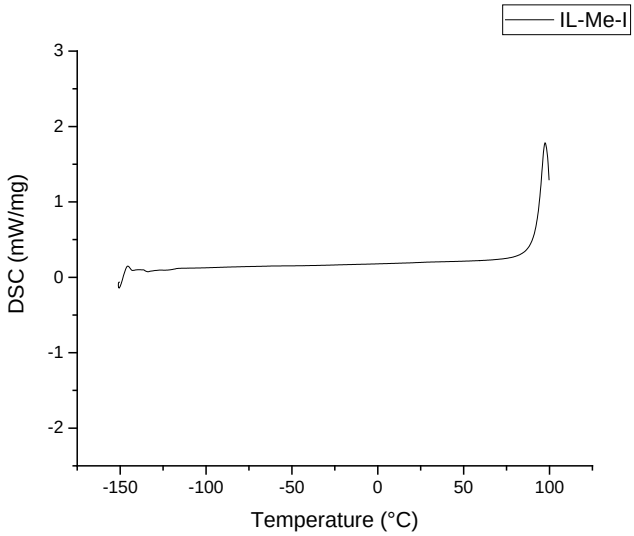


Glass transition: -85.5 °C, 0.255 J g^{-1} K^{-1},

Cold crystallization: -41.5 °C; -20.1 °C; -40.68 J g^{-1} (both together)

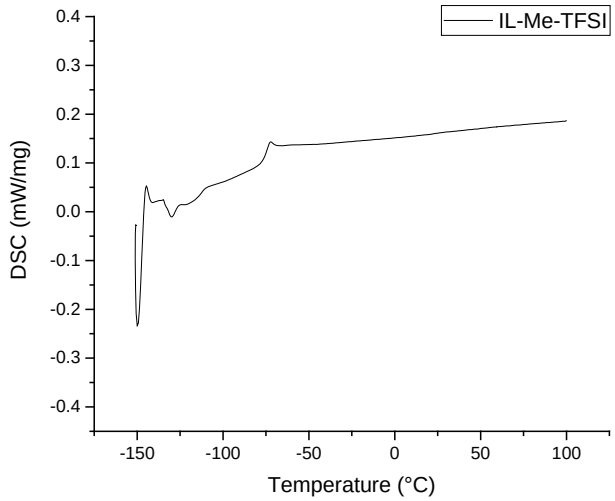
Melting: 1.3 °C, 40.86 J g^{-1}

1-Butyl-2,3-dimethylimidazolium iodide (IL-Me-I)



Melting could not be determined due to the measurement interval ending at 100 °C.

1-Butyl-2,3-dimethylimidazolium bis(trifluoromethanesulfonyl)imide (IL-Me-TFSI)

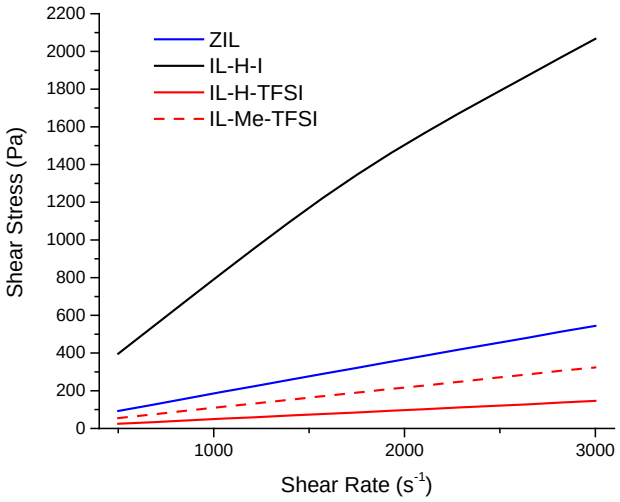


Glass transition: -75.4 °C, 0.195 J g^{-1} K^{-1}

Viscosity measurements

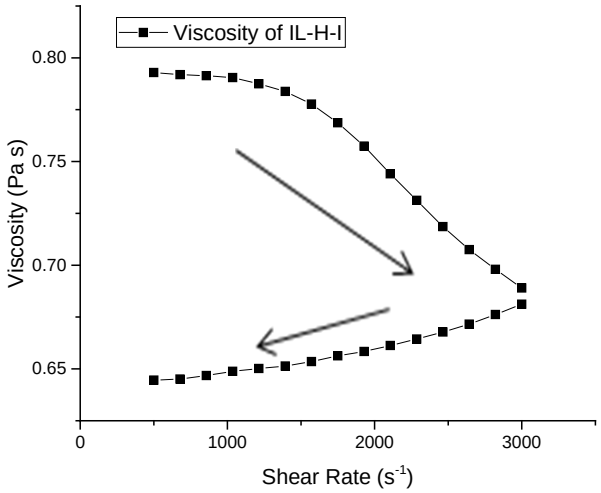
Dynamic viscosity was determined from the slope of a linear fit of shear rate – shear stress curves. All tested (zwitter)ionic liquids show Newtonian behavior. All tested liquid systems were dried extensively before measurement, however, measurements could not be performed under dry conditions, so ILs take up water from the atmosphere during measurement causing viscosity to decrease over time. The displayed measurements represent the first measurement cycle of a shear rate sweep from 500 to 3000 s^{-1}. In the case of the **ZIL**, additional measurements were performed after equilibration of the water content with the environment to illuminate the influence of water content.

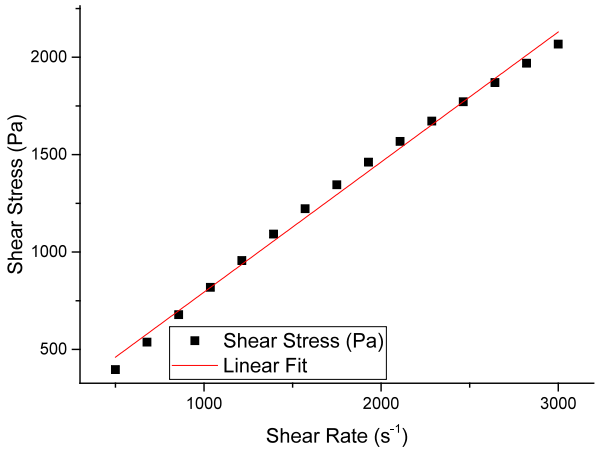
Shear stress–shear rate measurements



Up and down sweeps and linear regressions of up sweeps

1-Butyl-3-methylimidazolium iodide (IL-H-I)





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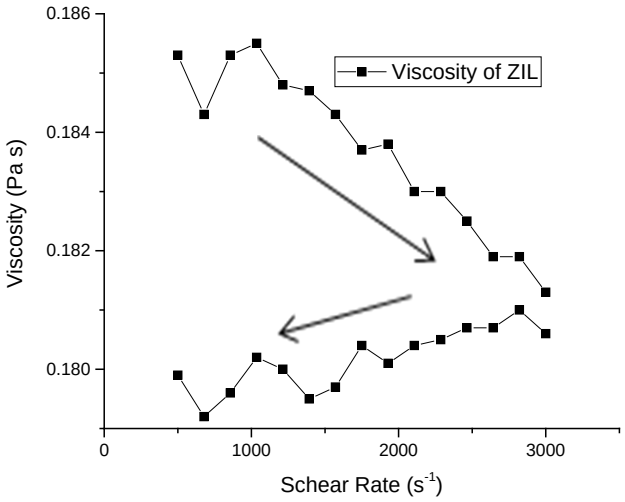
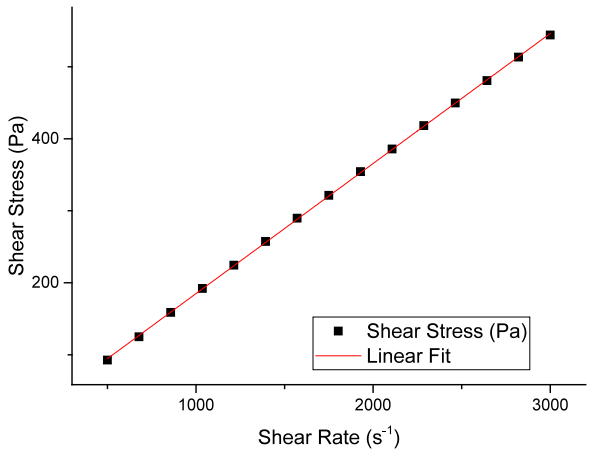
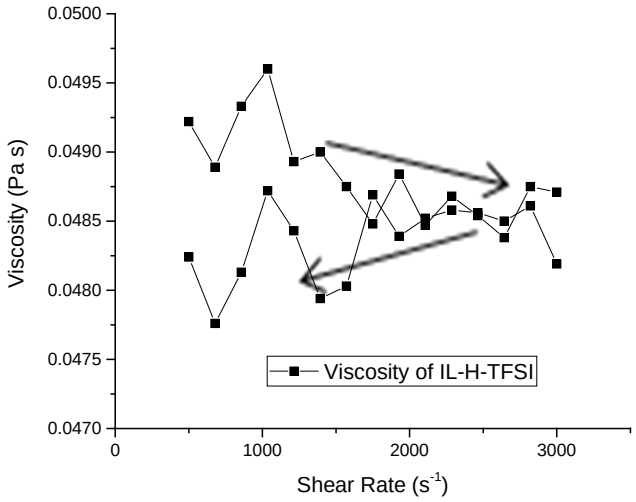
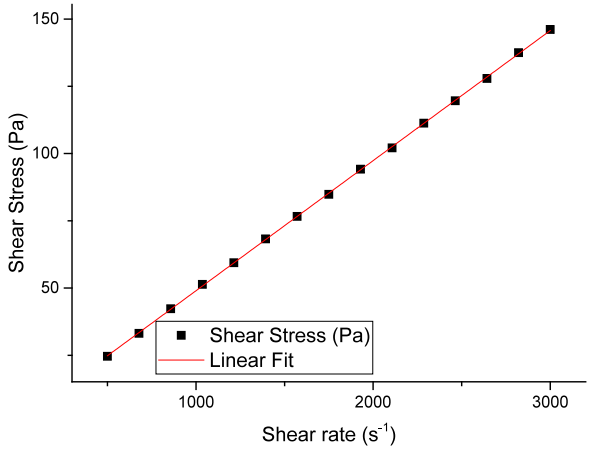


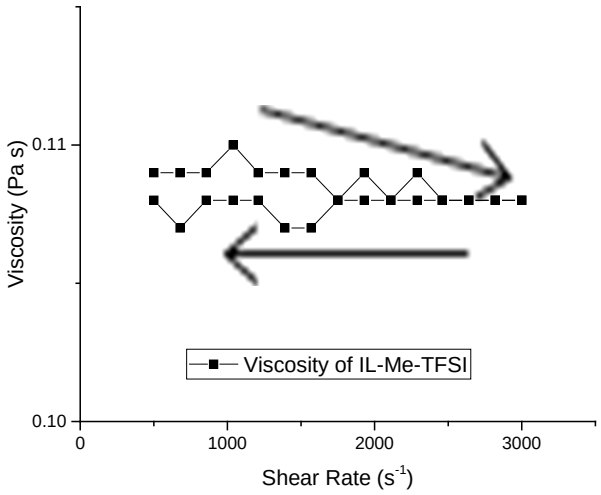


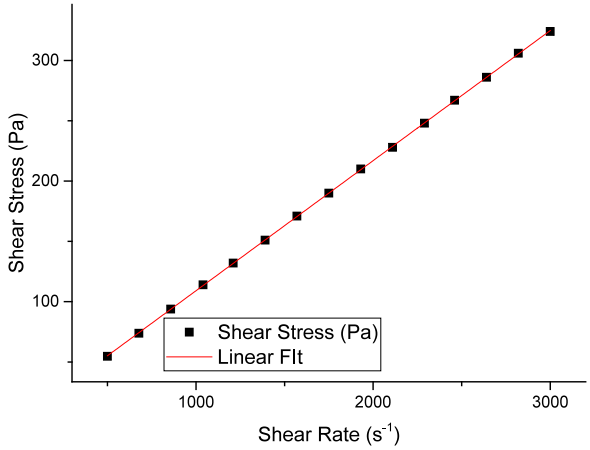
1-Butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide (IL-H-TFSI)



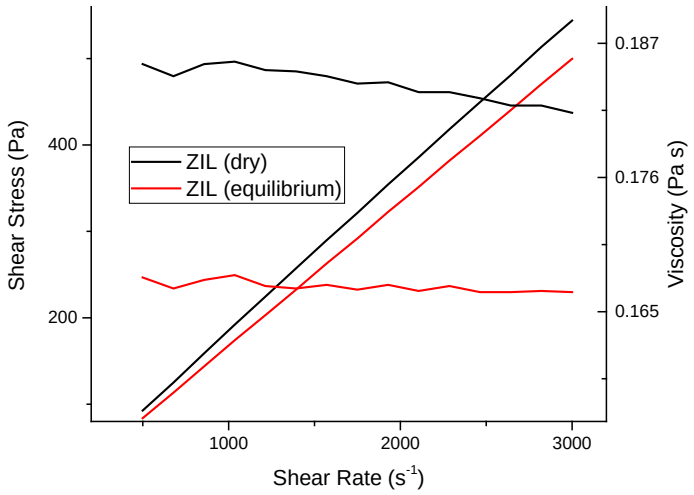


1-Butyl-2,3-dimethylimidazolium bis(trifluoromethanesulfonyl)imide (IL-Me-TFSI)





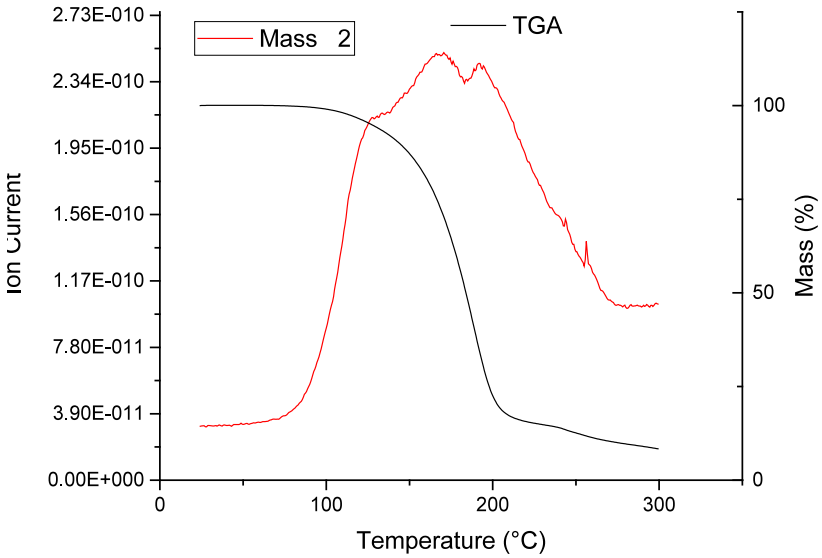
Equilibration of the ZIL with ambient humidity



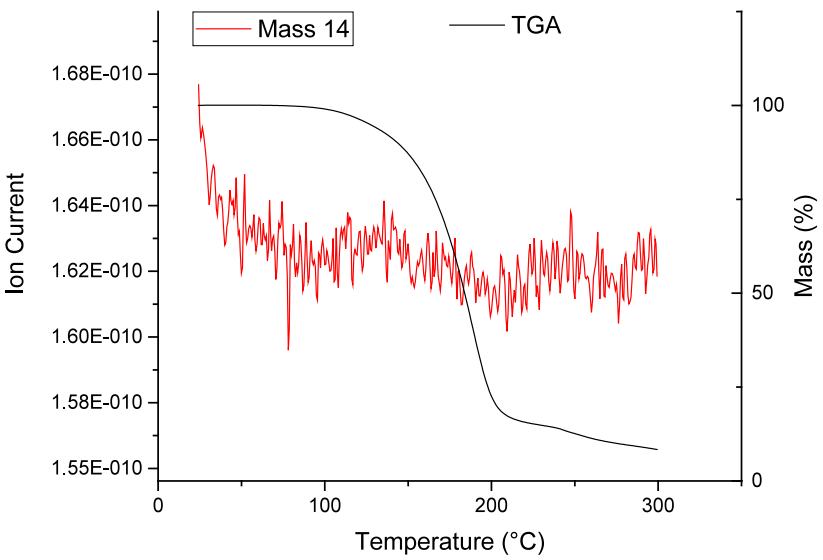
Thermal behavior and decomposition

Masses are rounded to the closest integer.

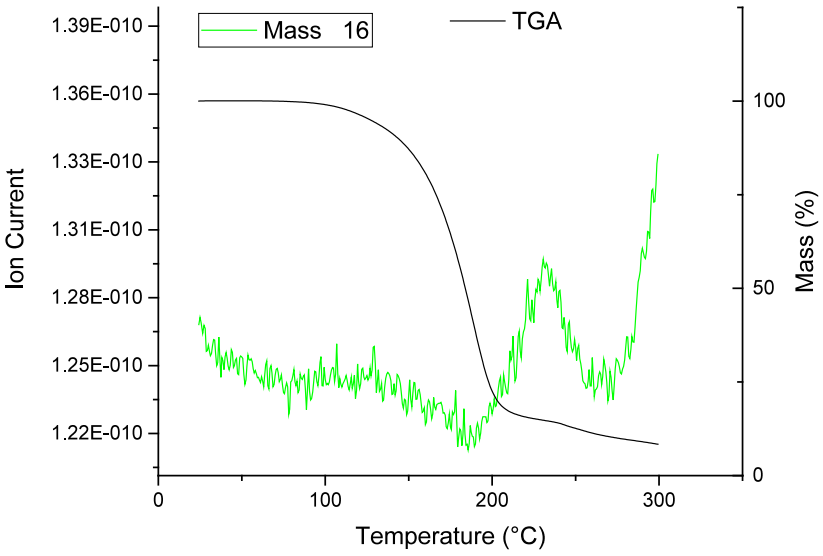
m/z 2



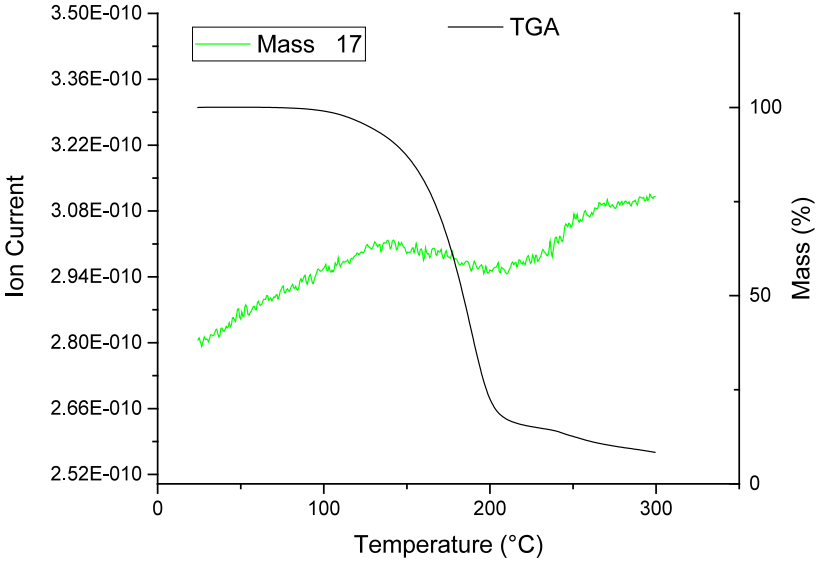
m/z 14


Mass 14
TGA
1.68E-010
1.66E-010
1.64E-010
1.62E-010
1.60E-010
1.58E-010
1.55E-010
Ion Current
100
50
0
Mass (%)
0
100
200
300
Temperature (°C)

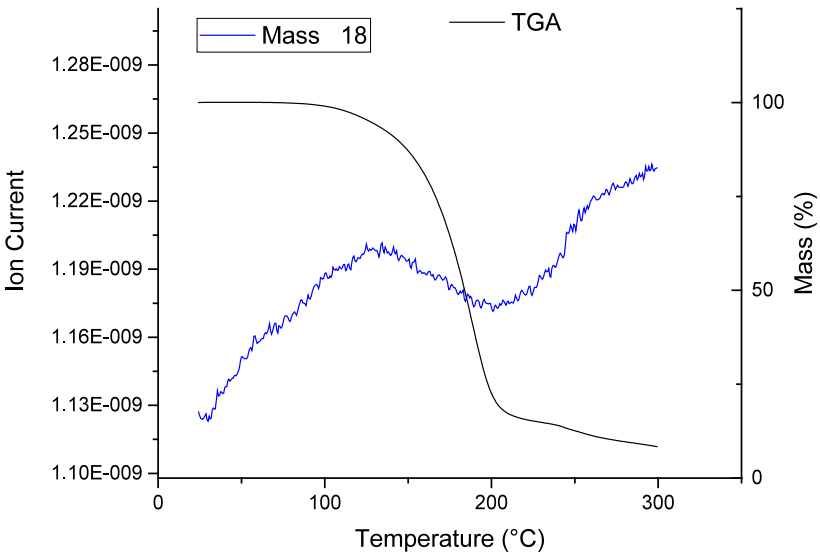
m/z 16


Mass 16
TGA
1.39E-010
1.36E-010
1.33E-010
1.31E-010
1.28E-010
1.25E-010
1.22E-010
Ion Current
100
50
0
Mass (%)
0
100
200
300
Temperature (°C)

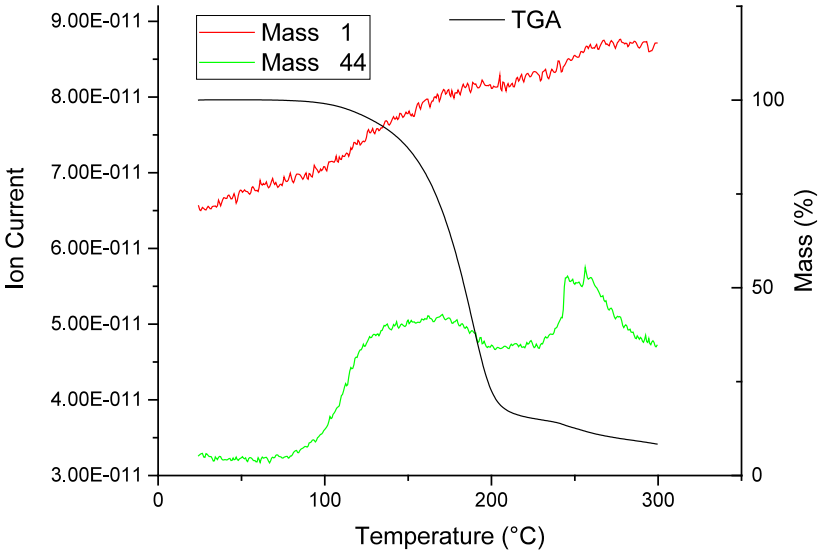
m/z 17


Mass 17
TGA
Ion Current
Mass (%)
Temperature (°C)
3.50E-010
3.36E-010
3.22E-010
3.08E-010
2.94E-010
2.80E-010
2.66E-010
2.52E-010
0
100
200
300
50

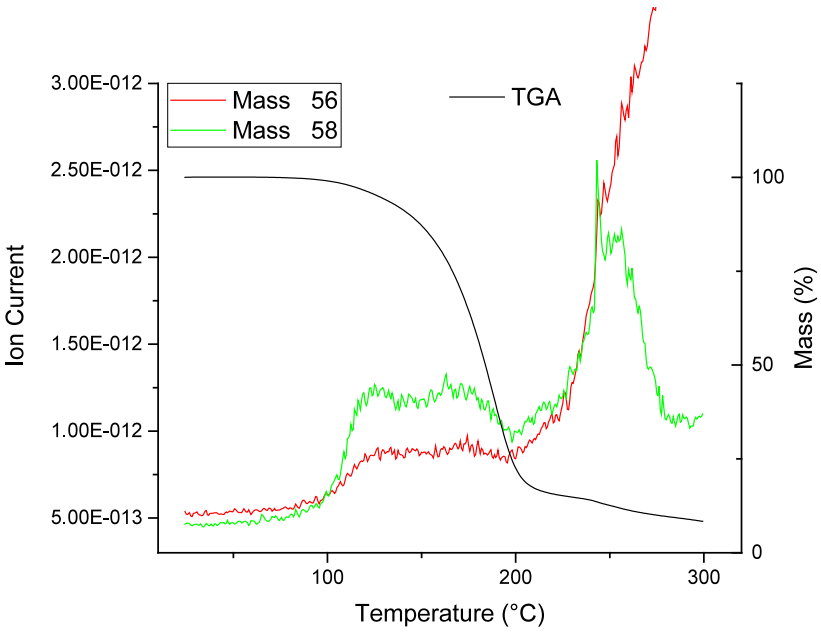
m/z 18


Mass 18
TGA
Ion Current
Mass (%)
Temperature (°C)
1.28E-009
1.25E-009
1.22E-009
1.19E-009
1.16E-009
1.13E-009
1.10E-009
0
100
200
300
50

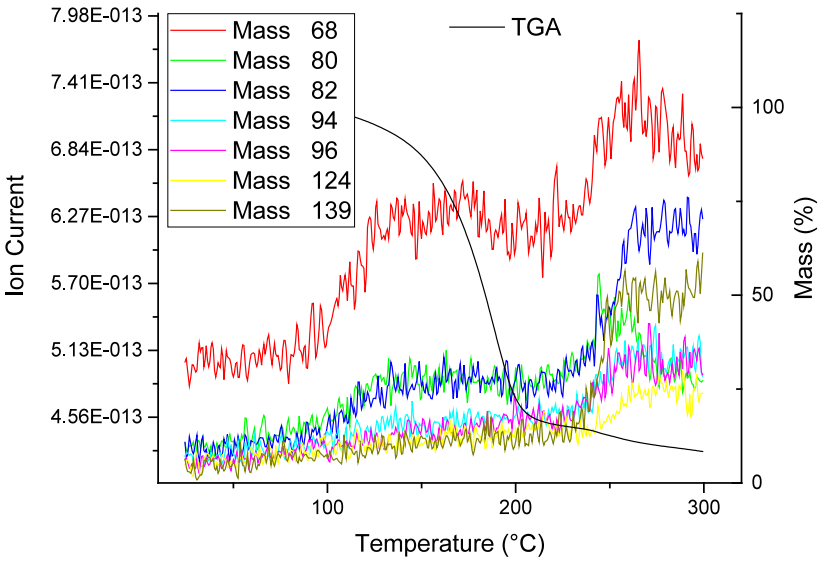
m/z 1; 44



m/z 56; 58



m/z 68; 80; 82; 94; 96; 124; 139



m/z 138; 154