Mass spectrometry-based methods for analysis of Ionic liquid species

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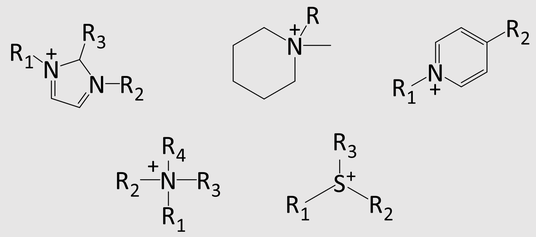
Ionic Liquids and Their Applications

Ionic liquids (ILs) are salts with low melting points, often defined as less than 100 °C.

Typically, ILs have bulky, asymmetric cations based upon one of a few common scaffolds.



The identity of the cation scaffold, cation substituent(s), and anion can be tuned for a variety of products and tasks.

While specific chemistry determines specific properties, as a class ILs often have properties including:

- Good thermal stability
- Non-volatility
- Good solubility in water
- High tunability
- Wide electrochemical window

These properties make ILs attractive for a wide range of (potential) applications.

Disinfectants and personal care products

Energy devices and applications

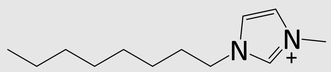
Chemical solvents

Space craft propellants

Potential Persistent Environmental Contaminants

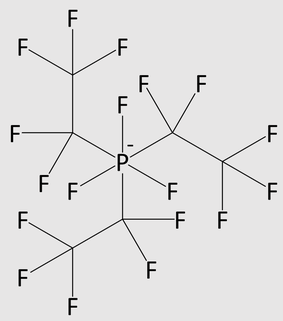
- As applications increase, possible point sources for environmental release also increase.
- Properties such as solubility, thermal stability and non-volatility make persistence in the environment, especially the aquatic environment, a possible concern.
- Environmental presence, bioaccumulation, toxicity, and related properties are subjects of ongoing investigations in environmental and analytical chemistry.
- Initial results suggest IL species are already in the environment.

3-methyl-1-octyl-1H-imidazole-3-ium (M8OI)



M8OI was detected in **soil** around a waste site (Probert et al., 2018) and in **human serum** (Leitch et al., 2021)

tris(pentafluoroethyl)trifluoro phosphate (FAP)



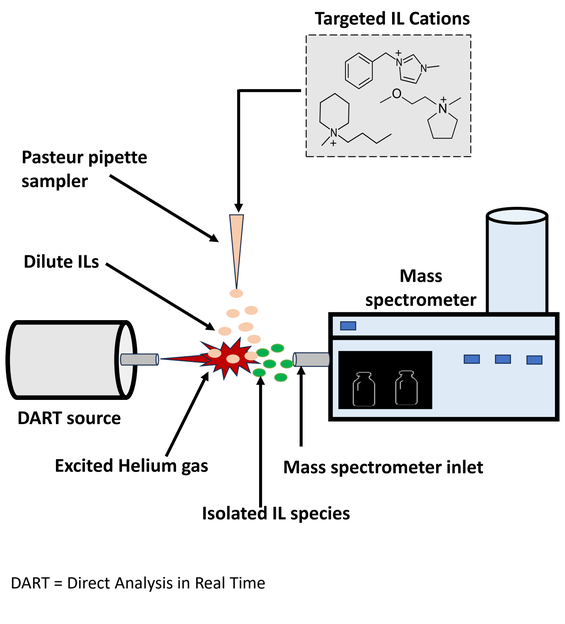
Neuwald et al., 2020, detected up to **3.4ug/L FAP** IL anion during screening of PFAS in **surface waters**

- Methods are needed to understand the scope of current contamination and to continue monitoring the situation in the future.
- For this, robust analytical methods for sample preparation and IL detection, characterization, and quantitation across many species is needed.

Mass Spectrometric Analysis of IL Species

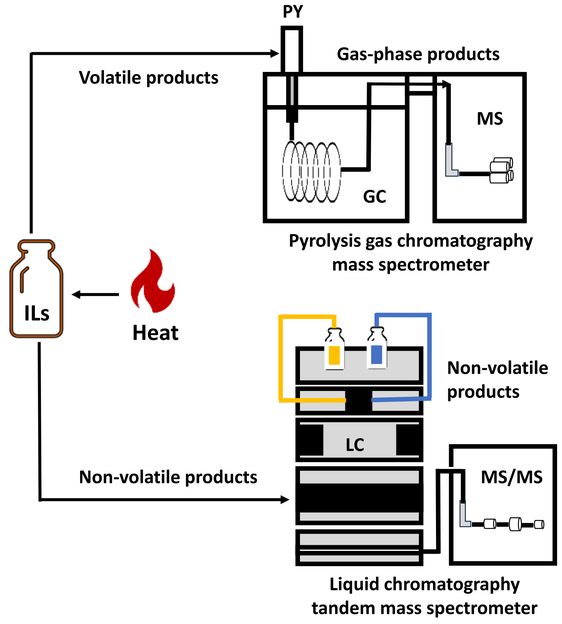
Mass spectrometers are versatile platforms suitable for the detection, characterization, and quantitation of various species. Given the fixed-charge nature of IL species, they should be readily amenable to analysis by mass spectrometry. Mass spectrometry is poised as a tool for applications as diverse as confirming the nature of synthetic IL species, monitoring degradation products from various stress conditions, detecting ILs from the environment, and more. Two example applications are shown below.

Rapid Screening for Known IL Species



DART = Direct Analysis in Real Time

Degradation Product Characterization



Relationship to Principles of Green Chemistry

1 2 3 4 5 6 7 8 9 10 11 12

1 Waste Prevention

ILs are recyclable, so research toward understanding IL properties especially decomposition temperatures and conditions, may improve recyclability.

3 Less Hazardous Chemical Synthesis

While ILs are typically non-volatile, many of their decomposition products are not. Better understanding IL stability and degradation products will help us understand and predict use conditions that minimize hazards and environmental threats of ILs.

10 Real-time analysis for pollution Prevention

Evaluating the analytical utility of DART-MS and other rapid screening methods moves us toward the goal of real-time, in process monitoring and possibly reduction of ILs in waste streams, as well as real-time monitoring of IL species present in the environment.

11 Design for Degradation

As a long-term potential impact, improved understanding of decomposition as a function of structure may eventually lead to rational design of ILs that can degrade completely into non-toxic products.

References

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