AccuTOF-GCv Series

Analysis of an Ionic Liquid by Using Field Desorption (FD) Ionization

Introduction
Ionic liquids are liquids that are predominantly comprised of ions and ion-pairs. More recently, this term has generally referred to salts that are in a liquid state at room temperature. Ionic liquids are electrically conductive and have an extremely low vapor pressure. Additionally, many of these liquids have low combustibility and excellent thermal stability. As a result of these properties, ionic liquids are expected to find many applications as functional materials.

In this work, we report the analysis of a commercially available ionic liquid by field desorption (FD) ionization using the JMS-T100GC “AccuTOF-GC” time-of-flight mass spectrometer.

Method
Sample: 1-Butyl-3-methylpyridinium bis(trifluormethylsulfonyl)imide (Aldrich part# 14654)

MS Conditions
Mass spectrometer: JMS-T100GC “AccuTOF GC”
Ionization mode: FD(+)
Cathode potential: -10 kV
Emitter current: 51.2 mA/min
Acquired mass range: m/z 35 – 800
Spectral recording interval: 1.0 sec

Results and Discussion
FD ionization is usually set up to observe positive ions; thus, the intact cation (C) is readily detected by this analysis. On the other hand, detecting the intact anion (A) alone tends to be fairly difficult. The former peak corresponds to the intact cation (C) whereas the latter peak corresponds to a cluster ion (CA+C). The results of accurate mass measurements for each ion are shown in Table 1.

Since the elemental compositions of C and CA+C were elucidated based on their exact masses, the elemental composition of A was derived as follows:

\[ A = (CA+C) - 2 \times C \]
\[ A = (C_{22}H_{32}F_{6}N_{3}O_{4}S_{2}) - 2 \times (C_{10}H_{16}N) = C_{2}F_{6}NO_{4}S_{2} \]

Conclusions
By using the AccuTOF-GC FD method to analyze ionic compounds, the intact cation can be readily detected, and the mass of the intact anion can be easily calculated using the cation mass and the cluster ion mass. Additionally, using the accurate mass measurements for the intact cation and the cluster ions, the elemental compositions of both the anion and cation can be easily elucidated for the ionic liquid.
References

3) MS Tips / Application Note for DART No.D031 (http://www.jeol.co.jp)