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)

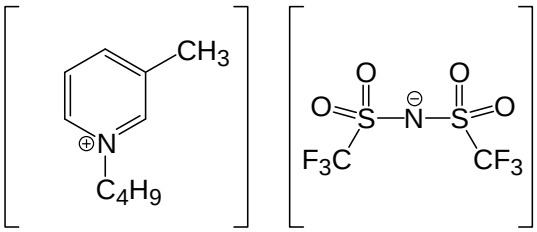

Fig. 1. Ionic liquid sample ions.

MS Conditions

Mass spectrometer: JMS-T100GC "AccuTOF GC"
Ionization mode: FD(+)
Cathode potential: -10 kV
Emitter current: 0 mA → 51.2 mA/min → 35 mA
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.[1, 2] For ionic compounds, single-charge cluster ions of the ($C_{n+1}A_n$) are readily observed by FD, but neutral species such as (CA) are not observed using this technique.[2] The acquired FD mass spectrum for the ionic liquid is shown in Fig. 2. The base peak was observed at *m/z* 150.1 and the second most abundant peak was observed at *m/z* 580.2.

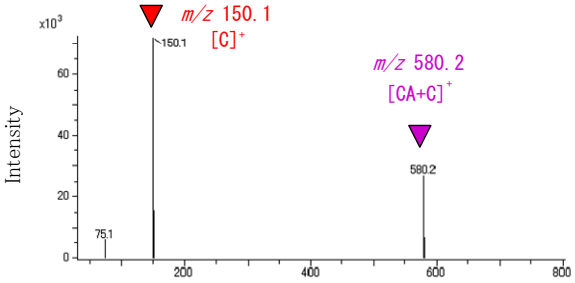

Fig. 2. FD mass spectrum of the sample

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.

Ionic species	Measured accurate mass	Calculated exact mass	Error (10^{-3} u)	Estimated formulae
C	150.1289	150.1283	0.6	$C_{10}H_{16}N$
CA+C	580.1766	580.1738	2.80	$C_{22}H_{32}F_6N_3O_4S_2$

Table 1. Measured accurate masses and calculated compositions of the ions.

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:

$A = (CA+C) - 2 \times C$

$A = (C_{22}H_{32}F_6N_3O_4S_2) - 2 \times (C_{10}H_{16}N) = C_2F_6NO_4S_2$

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.

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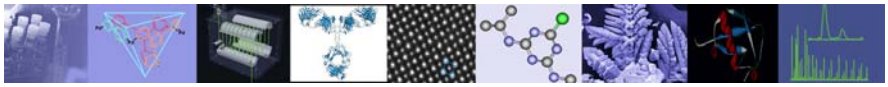

References

1) J. H. Gross, “Mass Spectrometry”, Springer-Verlag Berlin Heidelberg, Germany (2004).
2) J. H. Gross, *J. Am. Soc. Mass Spectrom.*, 18, 2254 (2007).
3) MS Tips / Application Note for DART No.D031 (http://www.jeol.co.jp)