JEOL MS Data Sheet

MS Tips

Mass Spectrometry Application Group
Mass Spectrometry Business Unit
JEOL Ltd.

No.113

Analysis of ionic liquid by field desorption (FD) ionization using JMS-T100GC "AccuTOF GC"

Introduction

Ionic liquids are liquids comprised predominantly of ions and ion-pairs. Recently, it has come to be used for salts that are in liquid state at room temperature. Ionic liquids are electrically conductive and have extremely low vapor pressure. Many have low combustibility and excellent thermal stability. They are expected to find many applications as functional materials.

Here we report the analysis of a commercially available ionic liquid by field desorption (FD) ionization using JMS-T100GC "AccuTOF GC" time-of-flight mass spectrometer.

Methods

Sample 1-Butyl-3-methylpyridinium bis(trifluormethylsulfonyl)imide (14654 Aldrich)

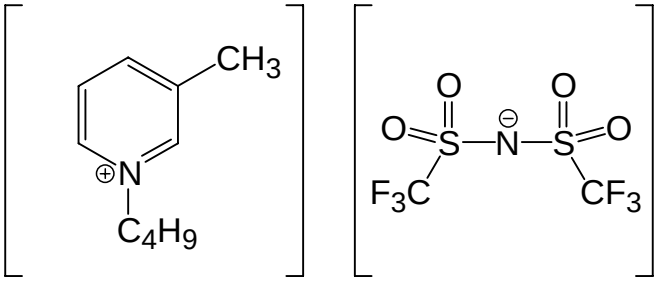

Fig. 1 Structural formula of the sample

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, the intact cation (C) is readily detected. On the other hand, detecting the intact anion (A) alone is difficult[1), 2)]. For ionic compounds, single-charge cluster ions of the ($C_{n+1}A_n$) are readily observed but neutral species such as (CA) are not observed[2)]. The acquired FD mass spectrum is shown in Fig. 2.

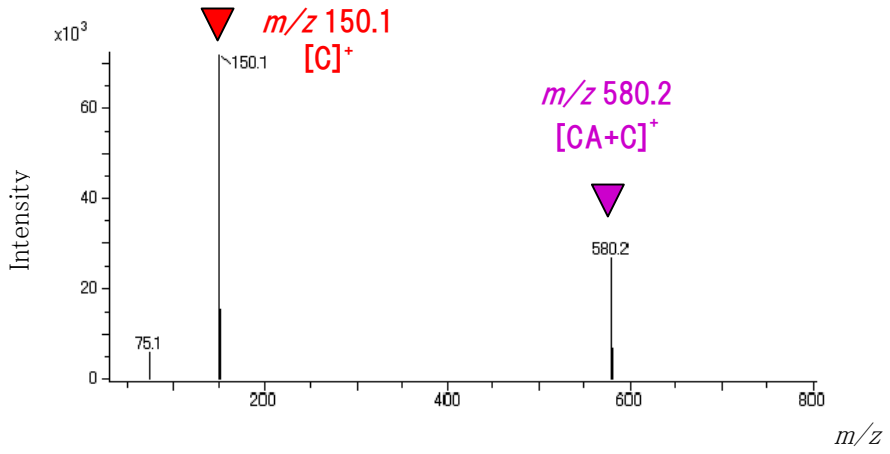

Fig. 2 FD mass spectrum of the sample

The base peak was observed at *m/z* 150.1 and the second most abundant peak was observed at *m/z* 580.2. The former corresponds to the intact cation (C) whereas the later corresponds to a cluster ion (CA+C). The results of accurate mass measurements of the ions are shown in Table 1.

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

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	$C_{22}H_{32}F_6N_3O_4S_2$

Since the elemental compositions of C and CA+C have been elucidated, the elemental composition of A can be derived:

(CA+C) – 2 x C = A

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

By analyzing ionic compounds by FD, the intact cation can be readily detected and the mass of the intact anion can be readily elucidated from the masses of the cluster ions. By measuring accurate masses of the intact cation and the cluster ions, the elemental compositions of both anion and cation can be elucidated.

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)