JEOL MS Data Sheet

MS Tips

Mass Spectrometry Application Group
Mass Spectrometry Business Unit
JEOL Ltd.

No.058

Accurate mass measurement of lube oil by GC/FI-TOFMS

FD (Field Desorption) and FI (Field Ionization) are ionization techniques based on the tunneling effect that is induced in high electric potential fields. When a sample is applied on the emitter in advance, it is called FD. On the other hand, it is called FI when a vaporized sample is introduced to the emitter.

FD and FI produces molecular ions easily and very few fragment ions. For this reason, FI is a very useful ionization method for samples which hardly produce molecular ions by EI (Electron Ionization), such as oil.

This application note shows the result of a commercial lube oil by GC/FI and the elemental composition determination by FI.

<Sample and measurement conditions>

Sample lube oil

Measurement conditions

For GC

GC:	Agilent 6890N
Column:	DB-5 (30m x 0.32 mm I.D., 0.25μm)
Oven temp.:	50C → 15C/min → 320C (2min)
Injection temp.:	280C
Injection amount:	1.0 μL [Split mode (1:200)]
Carrier gas:	He (Const. flow mode: 1mL/min)

For MS

MS:	JMS-T100GC “AccuTOF GC”
Ionization method:	FI (Cathode volt.: -10kV, Emitter current: 0mA)
Spectrum recording interval:	0.4 sec

<Result and discussion>

This sample was analyzed by GC/EI and hydrocarbons and fatty acid esters were determined.

Fig.1 shows TICC of lube oil by GC/FI. Hydrocarbons and fatty acid esters were observed in this TICC.

As an example, a mass spectrum of C13 hydrocarbon is shown in Fig.1. Only molecular ions are produced by FI. Since an exact mass of this molecular ion is known as 184.2191 ($C_{13}H_{28}$), this ion was used as internal calibrant in order to determine the elemental composition of other ions (peak1, 2, 3 and 4). The result of the elemental composition determination for other ions is shown in Table 1.

The accurate mass for all of molecular ions of peak 1, 2, 3 and 4 is within 2mDa from the exact mass.

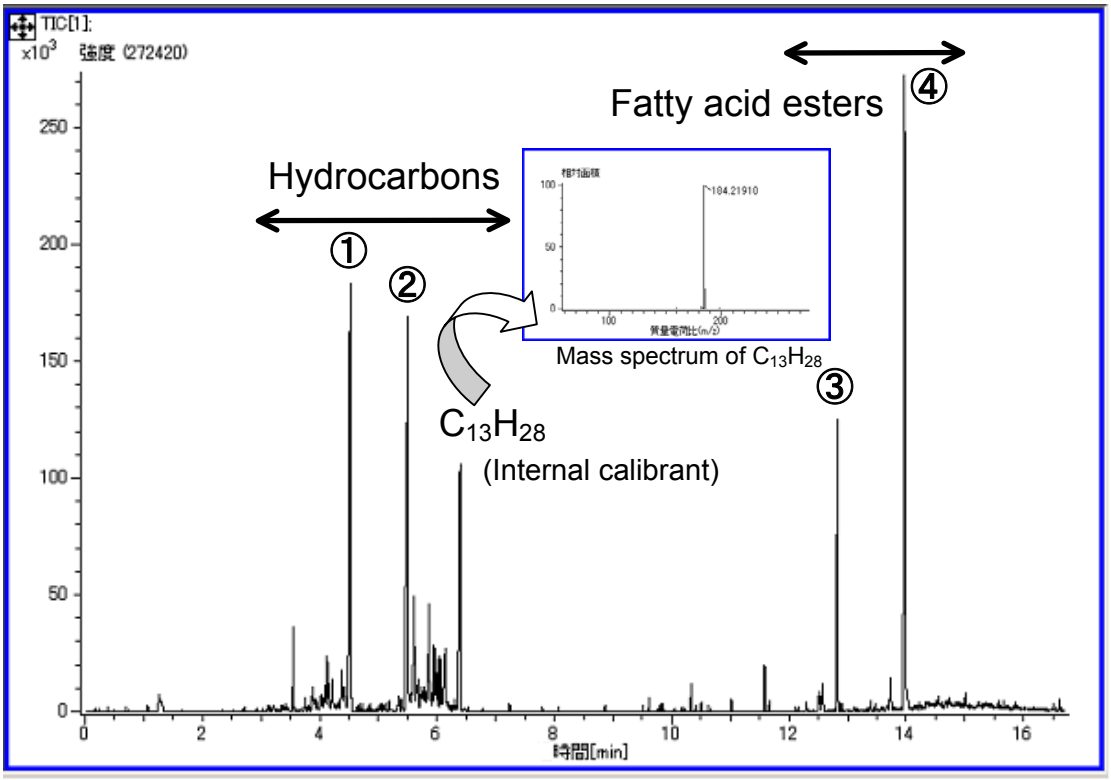

Fig.1 TICC of lube oil

Table 1 The result of elemental composition determination by GC/FI

	Cal. m/z	Obs. m/z	Diff.(mDa)	Formula
1	156.1878	156.1868	-1.0	$C_{11}H_{24}$
2	170.2034	170.2030	-0.4	$C_{12}H_{26}$
3	312.3028	312.3046	+1.8	$C_{20}H_{40}O_2$
4	340.3341	340.3356	+1.5	$C_{22}H_{44}O_2$

JMS-T100GC “AccuTOF GC” has essentially capabilities of high mass accuracy and very small systematic mass error. For this reason, AccuTOF GC can get accurate mass with single point internal calibrant by any kind of ionization method even by FI. Therefore, it is possible to perform elemental composition analysis with high reliability.