Analysis of Contaminants in Low Viscosity Solvents for Electrolytes in Liquid-LIB by GC-TOFMS

Product: Mass spectrometer (MS)

Introduction

The electrolyte in a lithium-ion battery (LIB) is made by dissolving the electrolyte in a liquid mixture of ethylene carbonate (EC) and various low-viscosity solvents. Producing a high purity electrolyte requires a high purity solvent and therefore it is important to have a good understanding of the composition of impurities in the solvent.JEOL's latest analytical software, msFineAnalysis AI, is designed for rapid analysis of GC-HRMS data acquired by both EI and SI, chemical formula determination, and chemical structure prediction. This application note reports a qualitative analysis of impurity components of dimethyl carbonate (DMC), which is commonly used as a solvent in electrolytes, as a case study of msFineAnalysis AI analysis.

Experiment

Commercially available DMC (≥98%) was used as the sample. The field ionization (FI) method was used as the EI method and SI, and msFineAnalysis AI was used for analysis. Details of the measurement conditions in the measurement are shown in Table 1.

JMS-T2000GC AccuTOF™ GC-Alpha High Performance GC-TOFMS

Table 1. Measurement and analysis conditions

GC-HRMS	
Gas Chromatograph	8890 GC (Agilent Technologies, Inc.)
Mode	Splitless
Inlet temperature	250 °C
Column	DB-5MS, 60m x 0.25mm, 0.25µm (Agilent Technologies, Inc.)
Oven	50°C (3min) →5°C/min →200°C (3min)
Carrier gas	He, 1.0mL/min
Injection volume	1µL
TOFMS	JMS-T2000GC (JEOL Ltd.)
Ionization	EI+ : 70eV, 300µA
	FI+ : -10kV, 12mA
Monitor ion range	*m/z* 29-800
Analysis software	msFineAnalysis AI (JEOL Ltd.)

Results and Discussion

The total ion current chromatogram (TICC) of EI is shown in Figure 1. The column bleed-derived siloxane and the main component, except DMC, were analyzed by msFineAnalysis AI as impurities. The TICC of EI and FI for the range analyzed by msFineAnalysis AI is shown in Figure 2. Impurities of 8 components were detected from the analysis range, and most of the components (ID[002]-ID[006], ID[008]) were identified with compound names and structural formulas with sufficient similarity by library search using the NIST database. For some compounds (ID[001], ID[007]) for which sufficient similarity could not be obtained by library search using the NIST database, the compound name and structural formula could be derived by structural analysis of msFineAnalysis AI. Figure 3 shows the candidate structural formula obtained from the AI structural analysis of ID[007].

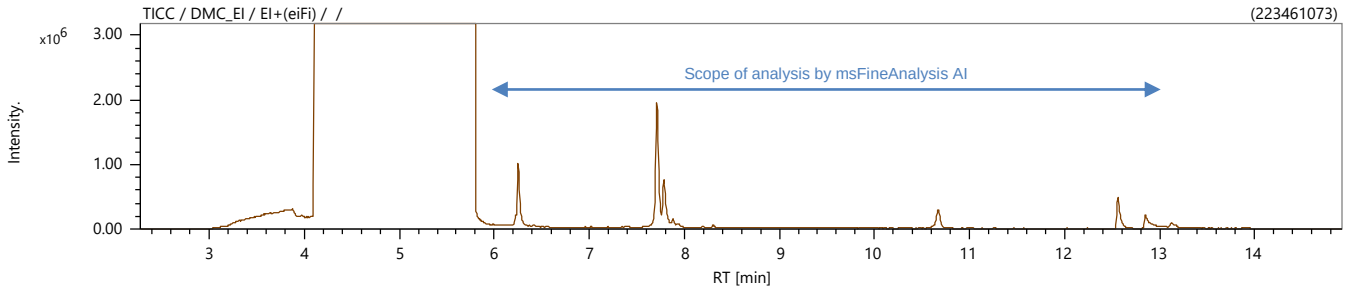

Figure 1. TICCs for ionization techniques EI.

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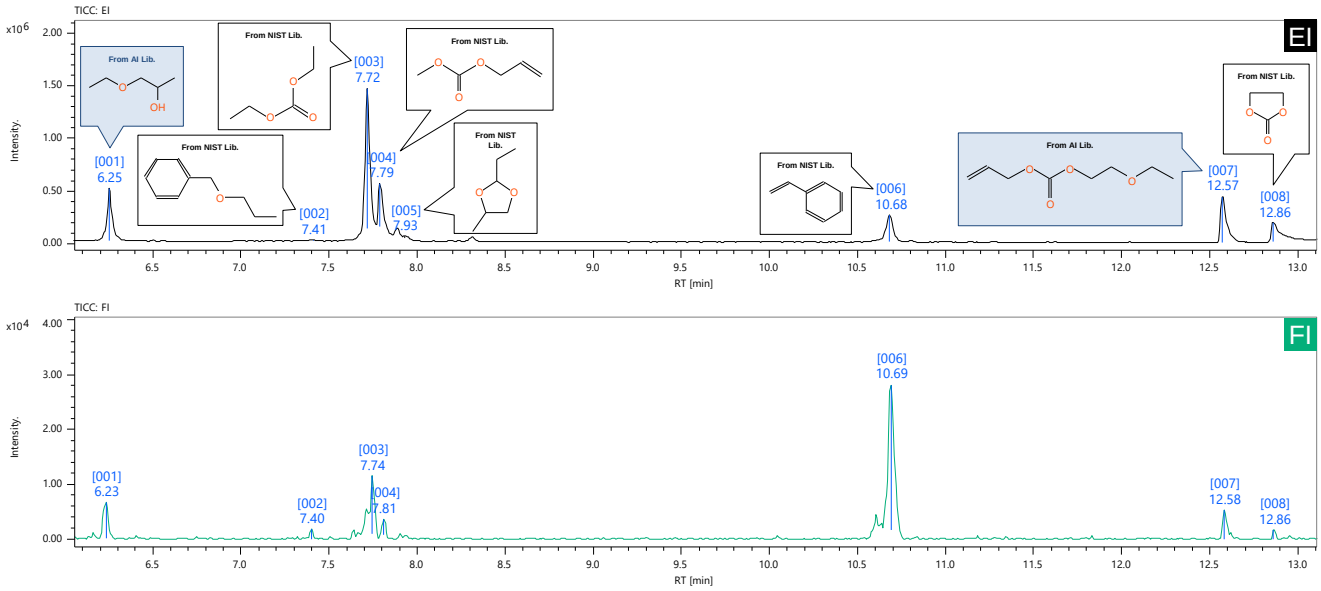

TICC for EI and FI methods with extended scope of msFineAnalysis AI analysis（Upper: EI, Lower: FI）.

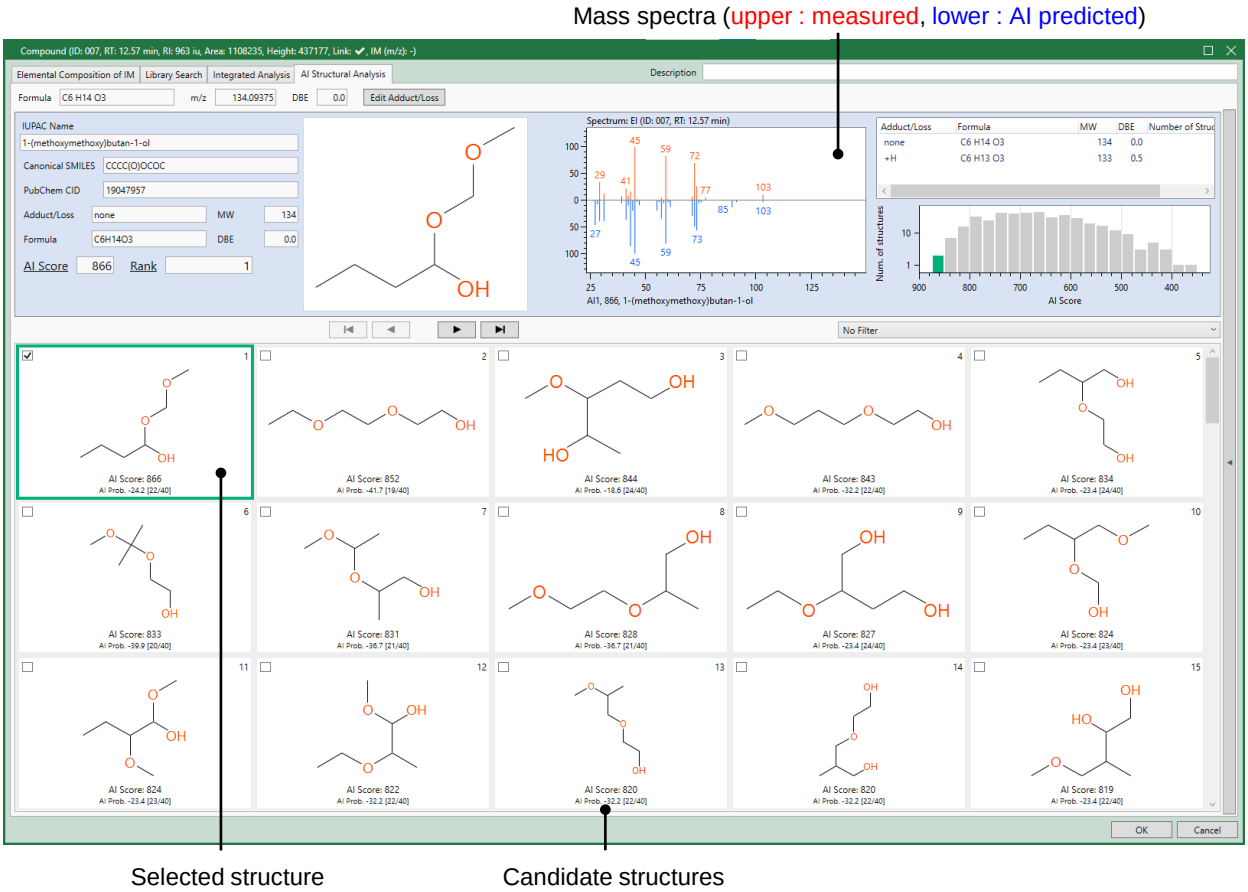

Figure 3. AI Structural analysis results of Peak ID [007].

Conclusion.

Impurities of DMC, which is commonly used as a solvent in electrolytic solutions, were measured by JMS-T2000GC and analyzed by msFineAnalysis AI, and as a result, DMC-like compounds such as Diethyl carbonate[003], Isobutylene carbonate[004], Ethylene carbonate[008] were detected as impurities. carbonate[004], and ethylene carbonate[008], which are compounds similar to DMC, were detected as impurities.

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