LAAN-A-LM-E046

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Application News

Liquid Chromatography Mass Spectrometry No.C75

Analysis of Impurities of Ru Dye (N719) for Dye-Sensitized Solar Cells

Solar cells are classified into several types, including a crystalline silicon type, a thin-film silicon type, a compound system type (CIGS, etc.), and the organic system type (organic thin-film type and dye-sensitized type), etc. Of these, about 90 percent of the solar cells being manufactured now are crystalline silicon solar cells. However, due to their manufacturing cost and the instability of a high-purity silicon supply, research and development of the next generation of dye-sensitized solar cell is being promoted.

The dye-sensitized solar cell is based on a system that generates electricity using dyes that are excited by light. This design has the advantages of high flexibility in determining color and shape, as well as low manufacturing cost. However, a variety of problems with this approach must first be addressed, including a solar conversion efficiency that is only about 1/3 that of the crystalline silicon type, and reliability (endurance), etc. In particular, even a minute amount of impurity in the dye will have a very adverse affect on the solar conversion efficiency. Here we introduce an example of the separation and qualitative analysis of impurities in the widely used dye, Ru N719, using the LCMS-2020.

*The Ru N719 dye was kindly provided by Dr. Liyuan Han of the NIMS-Advanced Photovoltaics Center in Ibaraki, Japan.

■ Flow Injection Analysis of N719 Using LCMS-2020

N719 is a dye with improved solar conversion efficiency which is derived from N3 by the bonding of tetrabutylammonium (TBA) at 2 of the carboxyl sites of the N3 dye. Fig. 1 shows the structure of N719. After dissolving the N719 sample in ethanol, ESI measurement was conducted. Fig. 2 shows the positive and negative mass spectra obtained. In the ESI positive mode, the tetrabutylammonium molecular ion was detected, while deprotonated molecules of compounds bonded with 0 to 3 tetrabutylammonium groups, as well as doubly-charged ions, etc. were detected using the ESI negative mode.

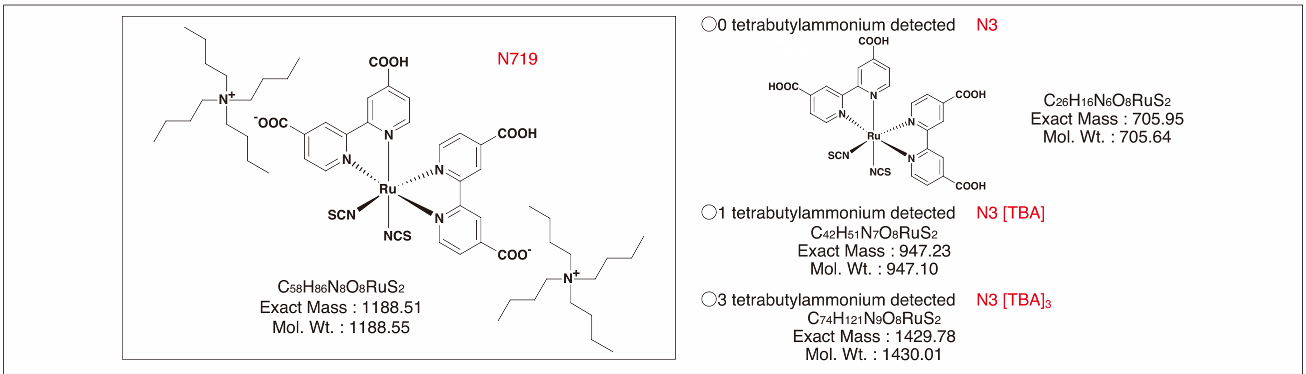

Fig. 1 Structure of N719

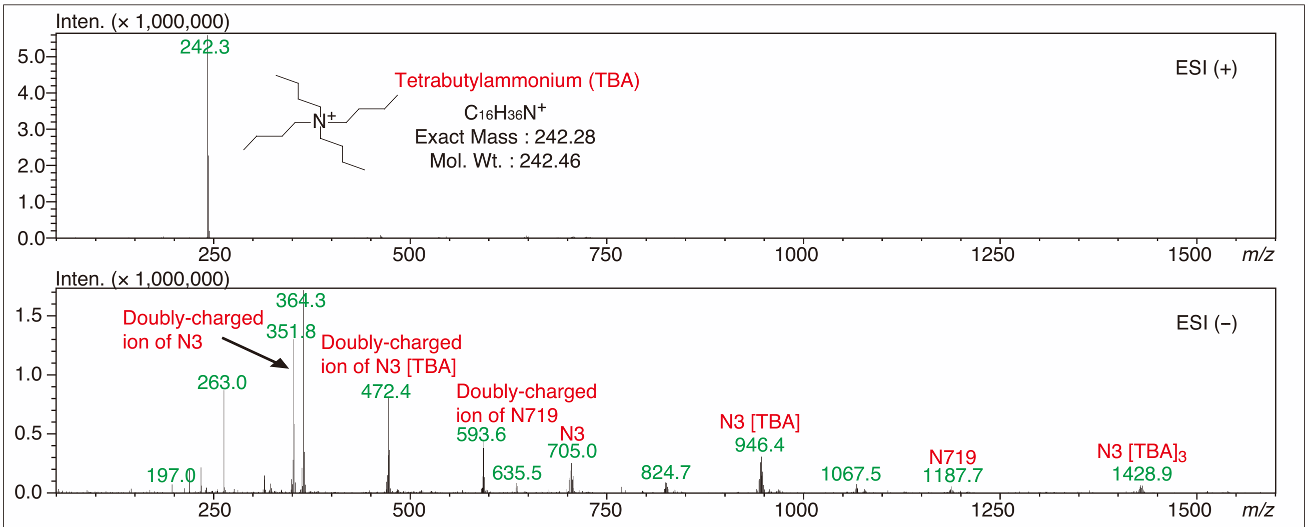

Fig. 2 FIA Mass Spectra of N719

■ Analysis of Impurities of N719 Using LCMS-2020

By conducting the analysis under acidic conditions, separation of N3 dye impurities having different structures at the X and Y sites was achieved. Fig. 3 shows the LC and MS chromatograms, and Fig. 4 shows the mass spectra at peaks A, B, F, and N3. Separation of N3 and compound F, which is difficult using the typical ODS column, was easily achieved using these conditions, demonstrating the ease with which quality control can be conducted.

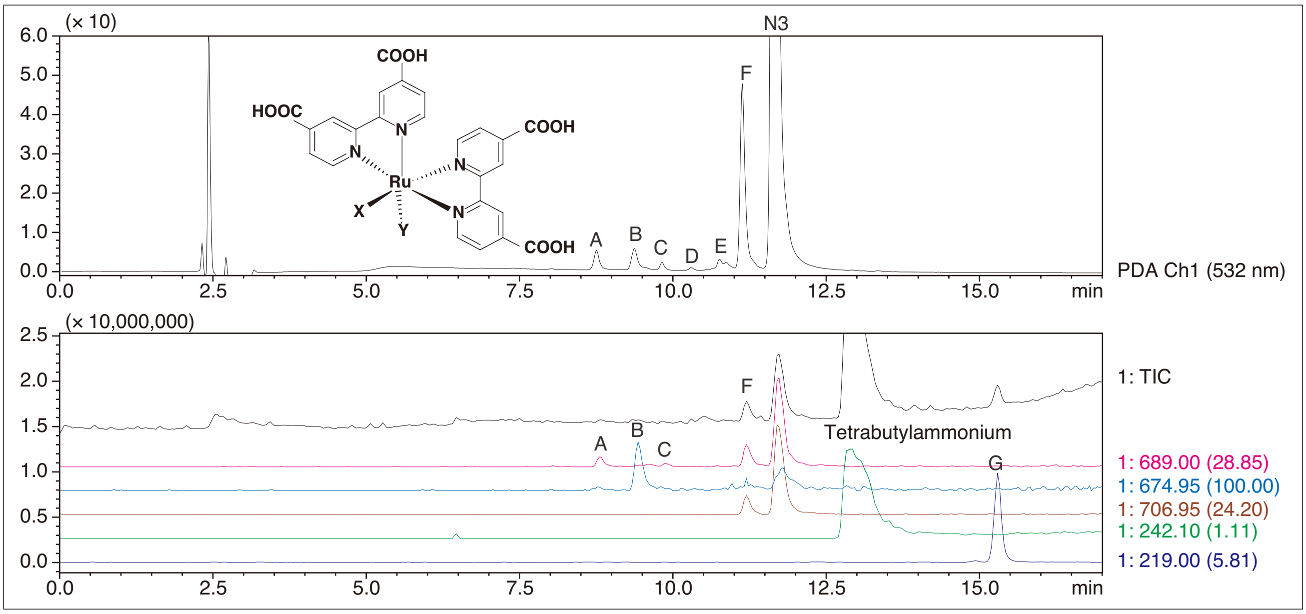

Fig. 3 Chromatograms of N719 in Ethanol Solution

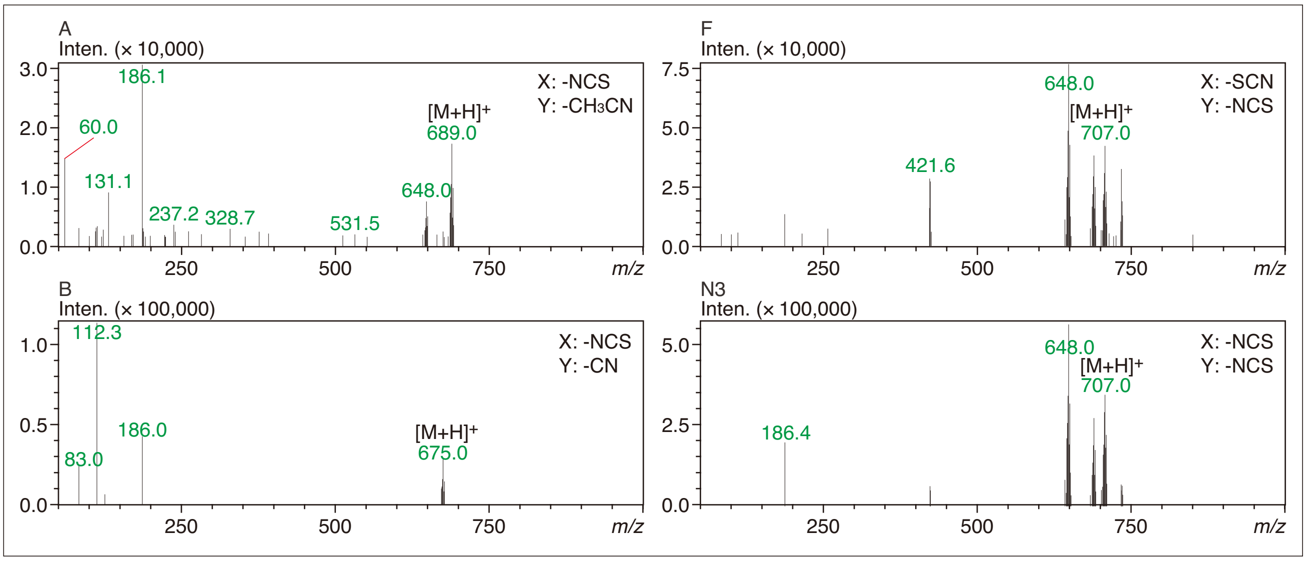

Fig. 4 ESI(+) Mass Spectra of Impurities A, B, F and N3

Table 1 Analytical Conditions for LC/MS

Column	: Phenomenex Fusion RP (150 mmL. × 2.0 mm I.D., 4 µm)	Probe Voltage	: +4.5 kV (ESI-Positive mode), -3.5 kV (ESI-Negative mode)
Mobile Phase A	: 1 % formic acid - water		
Mobile Phase B	: acetonitrile	Nebulizing Gas Flow	: 1.5 L/min
Gradient Program	: 5 %B (0 min) - 75 %B (15-20 min)- 5 %B (20.01 - 30 min)	Drying Gas Flow	: 10 L/min
Flow Rate	: 0.2 mL/min	DL Temperature	: 250 °C
Injection Volume	: 2 µL	Block Heater Temperature	: 450 °C
Column Temperature	: 25 °C	DL, Q-Array Voltages	: default values

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