

EO/PO composition ratio analysis of EO-PO copolymer using JMS-S3000 “SpiralTOF™-plus3.0” and “msRepeatFinder”

Related products: Mass Spectrometers (MS)

Ethylene oxide-propylene oxide (EO-PO) copolymer is one of copolymer type nonionic surfactants (nonionic surfactants) that combines hydrophilic EO and hydrophobic PO. It is used in various fields such as lubricants, antifoaming agents, emulsifiers, solubilizers, detergents, and antistatic agents. The physical properties of EO-PO copolymers are controlled by the sequence of EO/PO, such as random copolymerization or block copolymerization, and the number of added moles. MALDI is one of the typical soft ionization methods, and since ions derived from polymers are mainly singly charged ions, the m/z on the mass spectrum is the mass of the polymer ions. The use of high-mass-resolution MALDI-TOFMS makes it possible to easily identify polymer series due to differences in the composition of repeating units and end groups, and to calculate the molecular weight distribution of each. Using the KMD method, it became possible to easily visualize polymer series contained in complex high-mass-resolution mass spectra. In MSTips No. 423, structural analysis of EO-PO random copolymers and block copolymers was performed using matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOFMS) and solution nuclear magnetic resonance (NMR), complementary. As a result, similar values for the EO and PO composition ratio can be obtained when comparing the quantitative analysis of MALDI-TOFMS and NMR. In this application note, the EO/PO composition ratio using MALDI-TOFMS were investigated for the EO-PO copolymers with six different molecular weight distributions and EO/PO compositions.

Experiments

The six commercially available EO-PO copolymers (H/OH end-groups) were used as samples. In the MALDI-TOFMS experiment, DCTB was used as the matrix, and sodium trifluoroacetate (NaTFA) was used as the cationizing agent. The mass spectra were obtained using the SpiralTOF positive ion mode of JMS-S3000 “SpiralTOF™-plus3.0”. The mass spectra were deisotoped, and KMD analysis was applied using msRepeatFinder V7.

Table 1 Information of the six EO-PO copolymers

#	1	2	3	4	5	6
Average weight(M_n)	1100	1900	2000	2000	2700	2500
EO wt%	10.0	50.0	10.0	50.0	40.0	NA

Results

Figure 1 shows the mass spectra of six types of EO-PO copolymer. From the mass spectra, it is easy to confirm the molecular weight distribution. However, it is difficult to understand the composition ratio of EO/PO, Figure 2 shows the peak list after deisotoping in a KMD plot (Base unit PO).

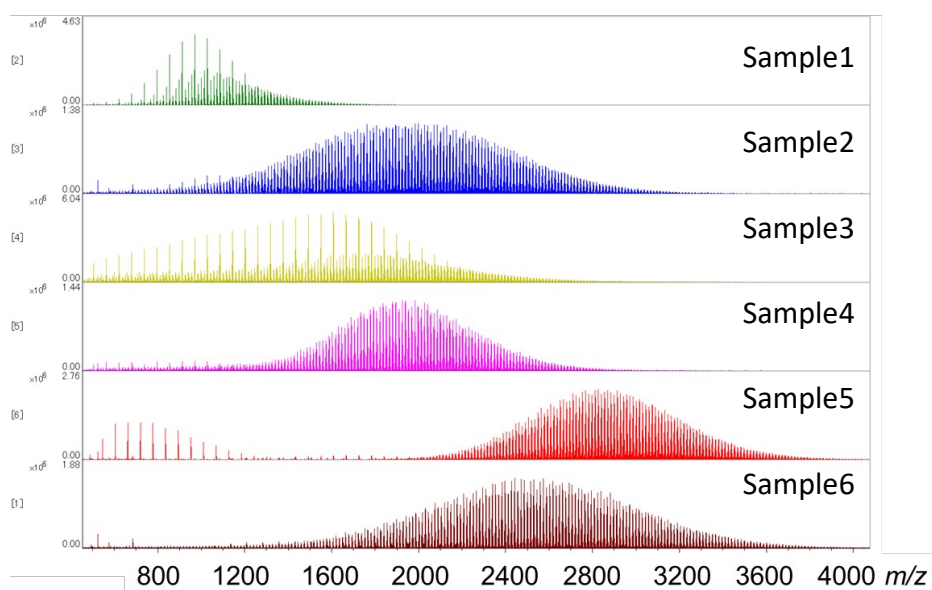


Figure 1 Mass spectra of six EO-PO copolymers.

KMDプロット Mr-58.04186 シフト:0.00

Distribution of EO

Distribution of PO

KMD

0.5

0.0

1000 2000 3000 4000 NKM

Figure 2 KMD plots (Base unit PO) of the six EO-PO copolymers after deisotoping the peak lists.

Table 2 Comparison of the EO weight ratios of the six EO-PO copolymers between the values in specification sheets and the values calculated from DP plots.

#	1	2	3	4	5	6
EO wt% (Specification sheet)	10.0	50.0	10.0	50.0	40.0	---
MALDI-TOFMS result	12.7	49.3	12.2	49.2	40.0	74.4

MALDI-TOFMS is a method that can quickly measure mass spectra, even including pretreatment. In recent years, the KMD analysis software msRepaetFinder, which facilitates high-resolution TOFMS data analysis of synthetic polymers, has enabled efficient analysis. In this report, we take these advantages to calculate the EO weight ratio, which is one of the important factors for EO-PO copolymers.

[1] MSTips 423 “Structural analysis of EO-PO copolymers using high-resolution MALDI-TOFMS and NMR”