●Identification of Surfactants

TNE0014

Overview

Surfactants, which are classified by polarity into cationic, anionic, and nonionic compounds, are added to a wide variety of products including industrial products like cleaning products and coating materials, medicine, and cosmetics. The following example describes how we analyze surfactants contained in commercial cleaning products.

Analysis Method

To analyze the structure of surfactants, its target compound is separated by solvent fractionation and ion-exchange treatment, and its structure is identified by instrumental analyses such as pyrolysis GC/MS (Py-GC/MS), NMR, and ESI-(APCI)-MS. If combined with polarity analysis, electron probe microanalysis (EPMA), and FT-IR, this type of structure analysis can be conducted more effectively.
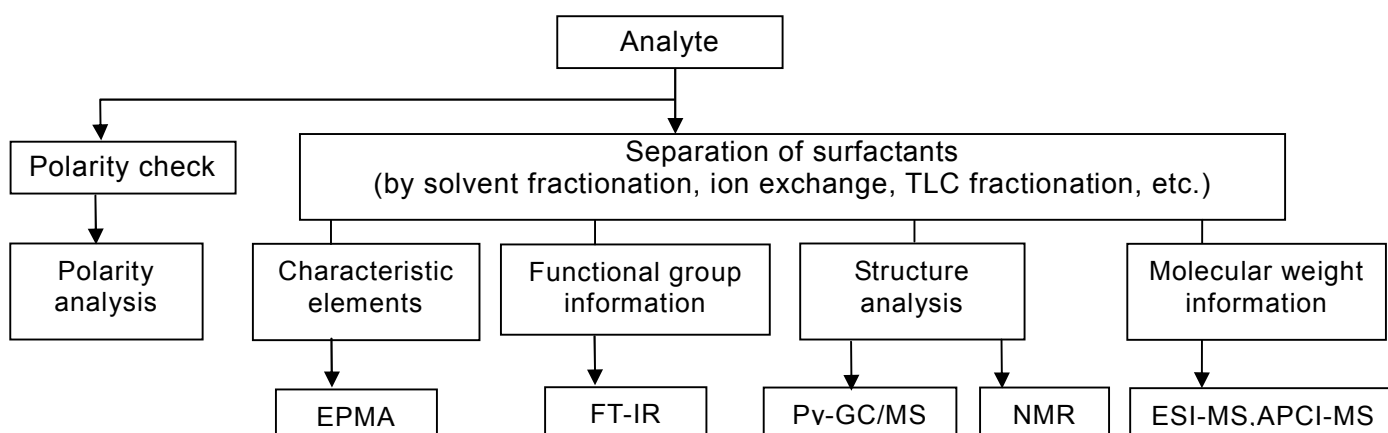
Figure 1: A scheme for analyzing surfactants

Analysis Example:

The solvent extract from the analyte was examined by Py-GC/MS, detecting a stearic acid analog and a polyethylene glycol oligomer (Figure 2). In addition, APCI-MS results showed the repeat unit m/z 44, indicating that the surfactant had a polyoxyethylene-like structure (Figure 3). Furthermore, the 1H NMR spectrum (Figure 4) provided information about the chemical bondinge of each component . As a result, the surfactant was estimated as polyoxyethylene monostearate (Figure 5).
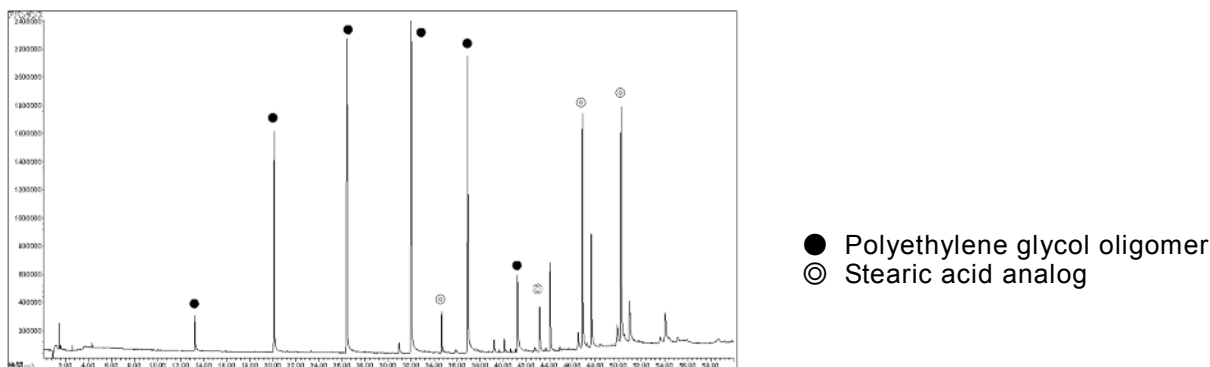
● Polyethylene glycol oligomer
◎ Stearic acid analog

Figure 2: Total ion current chromatogram by Py-GC/MS

Figure 3: APCI-MS (+) mass spectrum

Figure 4: 1H NMR spectrum

Polyoxyethylene monostearate where n = 4 to 12 (calculated from the molecular weight measured by APCI-MS)

Figure 5: Estimated structure of the surfactant