Structure Elucidation of Polyesters via Mass Spectrometry

Klara Saller, and Clemens Schwarzinger

Institute of Chemical Technology of Organic Materials, Johannes Kepler University, Linz, Austria

Since the 19th century polyesters of different kinds have played an important role in industry. The application of polyesters can be very versatile because their properties strongly depend on the type of monomers, their molar ratio and reaction conditions [1]. For the systematic development of polyesters for new applications, it is important to thoroughly investigate the polymer structure and its influence on the main properties.

Conventional methods of analyzing polyesters include gel permeation chromatography (GPC), and quantification of terminating groups (acid value and hydroxyl number) via titration. However, both methods combined still lack the ability to identify relations of number and kind of functionalities and chain length.

Therefore, synthesized polyesters are investigated by MALDI-TOF mass spectrometry (MS) which both reveals the structure of the polymer subunits and provides a molecular weight distribution. Additionally, the polymers can be fractionated by GPC and directly applied on MALDI targets to investigate certain molar mass regions separately. Figure 1 gives an example for structure elucidation using MALDI-TOF MS.



Figure 1: MALDI-TOF mass spectrum of a polyester.

^[1] U.Poth, *Polyester und Alkydharze*, 1st ed.; Vincentz Network: Hannover, Germany, 2005.