Application Note

Using Ion Mobility Mass Spectrometry to Separate Homopolymer Mixtures

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This is an Application Brief and does not contain a detailed Experimental section.

Abstract

This application brief decribes to separate a mixture of two homopolymers using ion mobility mass spectrometry on Waters SYNAPT G2 HDMS.

Benefits

The SYNAPT G2 HDMS with ion mobility functionality allows the separation of polymer mixtures.

Introduction

Mass spectrometry is a powerful tool for the polymer industry as it can be utilized to provide a range of vital information, including macromolecular connectivity, end group information, identification of monomer repeat units, and average molecular weight. This information can be used to indicate the manufacturing process used and the physical properties of the polymer.[1]

Synthetically manufactured polymers contain a range of molecular weight molecules, therefore many ions are observed when they are analyzed by mass spectrometry. If there are two homopolymers present it may become increasingly difficult to interpret the data due to the overlap of polymer ion series, especially if multiple charging has occurred. The additional orthogonal separating power offered by ion mobility (IM) provides a valuable tool for analysts. Figure 1 shows a mass spectrum and IM drift time plot of a polymer mixture containing poly ethylene glycol (PEG) and poly methyl methacrylate (PMMA).

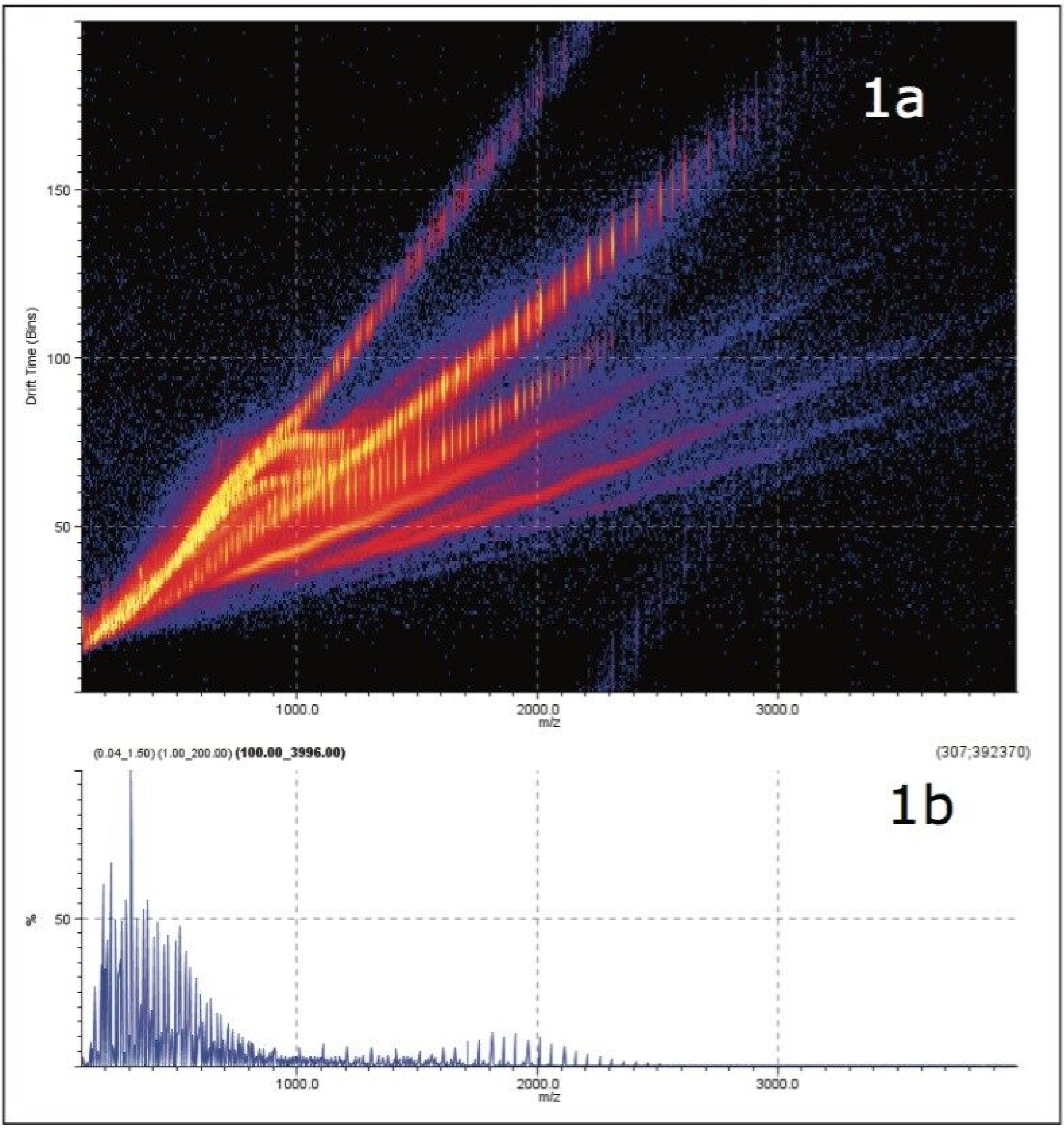

Figure 1. DriftScope data of 20 ppm PMMA 4000 and 20 ppm PEG 3000. (1a) IM drift time plot and (1b) mass spectrum.

Results and Discussion

Data were collected by infusing a sample containing a mixture of two polymers, poly methyl methacrylate (PMMA) 4000 and poly ethylene glycol (PEG) 3000, into Waters SYNAPT G2 HDMS with electrospray ionization and ion mobility enabled.

A high cone voltage was set to reduce multiple charging of the polymers making a doubly charged series of PMMA *m/z* 2000 relatively simple to identify. Confident identification of the PEG present would be very difficult without the mobility data due to the overlap of PEG and PMMA ion series, the complexity of which was increased due to multiple charging.

DriftScope Software was used to view the mobility data. Within DriftScope, a tool was utilized that allows data points to be selected and interpreted separately from the whole data set. Peak detection on the drift time plot was also used, identifying ions over a selected threshold, making it easier to identify ion series. Figure 2 shows the IM drift time plot and extracted spectra of PEG and PMMA. Highlighted are the areas within the mobility data that have been selected to generate the two spectra, confirming the presence of two polymers.

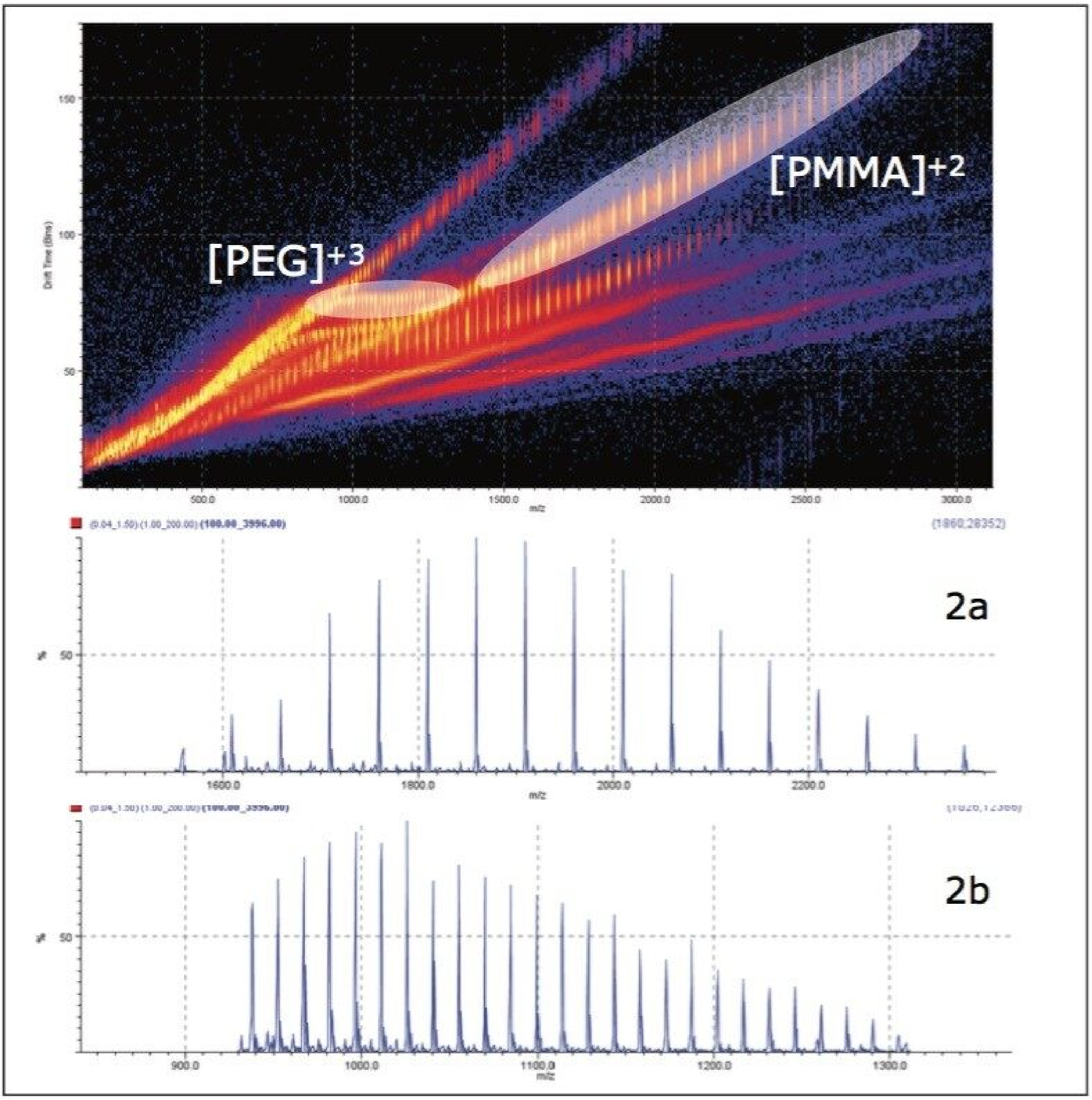

Figure 2. IM drift time plot of the polymer mixture. Highlighted are the select data points used to generate the two spectra shown (2a) PMMA 4000 and (2b) PEG 3000.

If additional confirmation or structural information is required, collision energy can be applied both before and/or after the mobility cell allowing true MS/MS analysis to be carried out.

Conclusion

The SYNAPT G2 HDMS offers robust exact mass data and orthogonal separation by ion mobility. This separates molecules by their shape, size, conformation, and mass-to-charge ratio. This is a powerful tool when analyzing complex samples such as polymer mixtures.

DriftScope Software has many tools to help analysts interrogate complex data, including multiple ways to view the data and peak detect ions, allowing ion series and related ions to be more easily identified. Selected data can be extracted and viewed in isolation to reduce the complexity, increase confidence, and allow faster data interpretation.

References

1. A T Jackson, K Thalassinos, R O John, N McGuire, D Freeman, J H Scrivens. *Polymer* 51: 1418-1424, 2010.

720004342, May 2012