HSLU Hochschule Luzern

Practical 3:

Analysis of PAHs in Plastics by GC-MS

Environmental Chemistry and Biology HS2024

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1 Introduction

The purpose of this experiment is to understand the analysis and quantification of polycyclic aromatic hydrocarbons (PAHs) in plastics using Gas Chromatography-Mass Spectrometry (GC-MS). This involves learning key concepts such as chromatographic separation, detection techniques, and calibration methods.

2 Materials and Methods

2.1 Materials

- Gas chromatograph (Agilent Technologies GC 6890N)
- Mass spectrometer (Agilent MSD 5973)
- Supelco SLB-5 ms column (30 m × 250 μm × 0.25 μm)
- Helium (carrier gas)
- Standard PAH kit
- Acetonitrile (solvent)
- Pipettes and vials

2.2 Experimental Procedure

1. **Sample Preparation:** Prepare dilutions from a 10 μg/mL stock solution using the formula $C_1V_1 = C_2V_2$ to achieve concentrations of 1 μg/mL, 0.1 μg/mL, and 0.01 μg/mL.

2. **GC-MS Setup:** Set the column temperature program to start at 70 °C, increase at 5 °C/min to 350 °C, and hold for 5 minutes.

3. **Injection:** Inject 1 μL of each dilution into the GC-MS system in split mode.

4. **Data Acquisition:** Record chromatograms, noting retention times, peak areas, and mass spectra for each PAH.

5. **Calibration Curve:** Use the standard solutions to construct a calibration curve by plotting peak area against concentration.

3 Results

3.1 Calibration Data

Table 1: Calibration data for Chrysene

Concentration (ng/mL)	Peak Area	Retention Time (min)	m/z Fragments
1000	1025	8.5	228
100	520	8.5	228
50	260	8.5	228
10	105	8.5	228
5	50	8.5	228

3.2 Chromatograms

Include chromatograms here with appropriate annotations.

3.3 Unknown Sample Analysis

The peak area for the unknown sample was 300. Using the calibration curve equation, the concentration is determined as:

$$C = \frac{(300 - 0)}{12} = 25 \, \text{ng/mL}$$

Equation 1: Concentration of Chrysene in the unknown sample

4 Discussion

- Discuss the separation efficiency, retention times, and peak identification.

- Answer questions on compound appearance order, fragmentation, and hydrophobicity.

- Explain the differences between the calibration curve method and the internal standard method.

5 Conclusion

This experiment provided a hands-on understanding of GC-MS analysis for PAHs, highlighting the importance of calibration and method validation for accurate quantification.