HSLU Hochschule Luzern

Practical 3:

Analysis of PAHs in Plastics by GC-MS

Environmental Chemistry and Biology HS2024

Dr. Macarena San Martín Ruiz
Lecturer

Team 4
Matteo Frongillo
Ramadhan Nura
Folagbade Popoola
Jonathan Lawrence Boms
Kron Xhemajli

Contents

1 Introduction **3**

2 Materials and Methods **3**
2.1 Materials . . . 3
2.2 Experimental Procedure . . . 3
2.3 Preparation of diluted solutions for a calibration curve . . . 3
2.3.1 Legend . . . 3
2.3.2 Formulas . . . 3
2.3.3 Ratios . . . 3

3 Results **4**
3.1 PAHs detected . . . 4
3.1.1 LMW PAHs . . . 4
3.1.2 HMW PAHs . . . 4
3.1.3 Data sheet . . . 4
3.2 Chromatograms . . . 5
3.3 Unknown Sample Analysis . . . 5

4 Discussion **5**

5 Conclusion **5**

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 – Mass spectrometer
- Helium (carrier gas)
- Standard PAH kit
- Chloroform (solvent)
- Vials
- Pipettes

2.2 Experimental Procedure

2.3 Preparation of diluted solutions for a calibration curve

2.3.1 Legend

- $\mathbf{C_i}$: Initial stock concentration (μg/mL)
- $\mathbf{C_t}$: Target concentration (μg/mL)
- $\mathbf{V_s}$: Volume of stock solution required (mL)
- $\mathbf{V_t}$: Target volume (mL)
- $\mathbf{V_c}$: Volume of chloroform required (mL)

2.3.2 Formulas

- Amount of volume of stock solution required $\mathbf{V_s}$:

$$V_s = \frac{C_t \cdot V_t}{C_i}$$

Equation 1: Stock solution volume

- Volume of chloroform required $\mathbf{V_c}$:

$$V_c = V_t - V_s$$

Equation 2: Solvent volume

2.3.3 Ratios

Table 1: Diluted solution ratios

Dilution	$\mathbf{C_i}$	$\mathbf{C_t}$	$\mathbf{V_s}$	$\mathbf{V_t}$	$\mathbf{V_c}$
1:10	10	1	0.1	1	0.9
1:100	10	0.1	0.01	1	0.99
1:1000	10	0.01	0.001	1	0.999

3 Results

3.1 PAHs detected

3.1.1 LMW PAHs

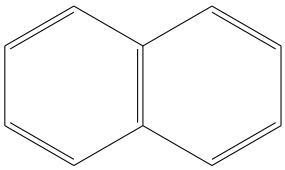

Figure 1: Naphtalene

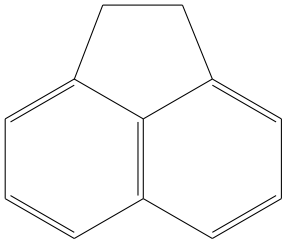

Figure 2: Acenaphthene

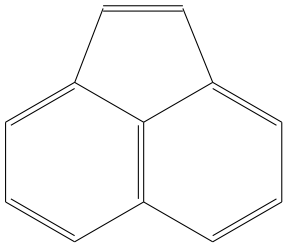

Figure 3: Acenaphthylene

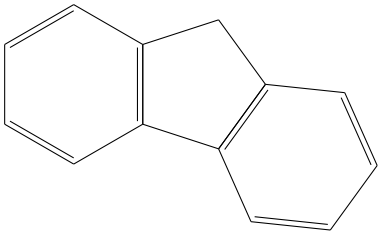

Figure 4: Fluorene

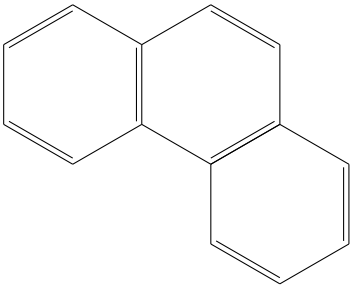

Figure 5: Phenanthrene

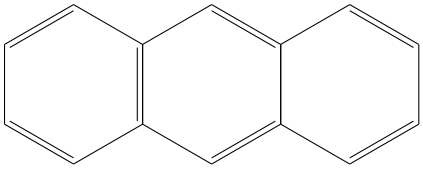

Figure 6: Anthracene

3.1.2 HMW PAHs

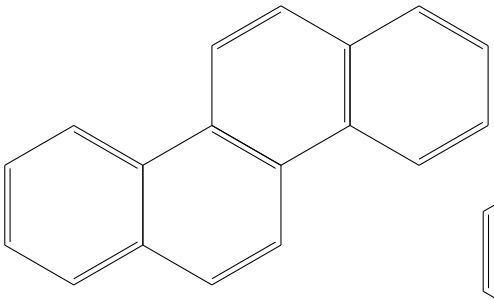

Figure 7: Chrysene

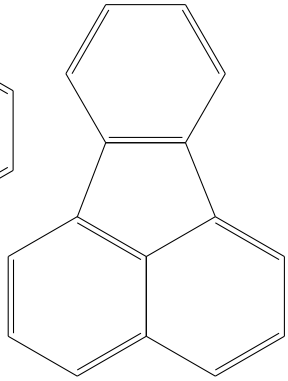

Figure 8: Fluoranthene

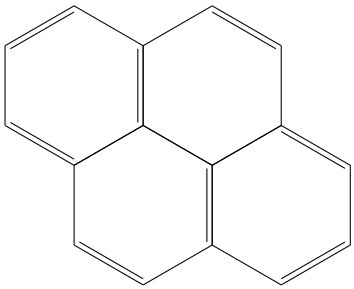

Figure 9: Pyrene

3.1.3 Data sheet

Table 2: Compounds data

Nr.	Compound name	Concentration (ng/mL)	Retention time	Peak area	m/z fragments
1	Naphtalene		4.62	938975	128
2	Acenaphthylene		7.78	1093694	152
3	Acenaphthene		8.18	1306917	154
4	Fluorene		9.35	1134899	166
5	Anthracene		11.58	1115451	178
6	Phenanthrene		11.71	N.D.	178
7	Pyrene		14.46	1358324	202
8	Fluoranthene		15.00	1533223	202
9	Chrysene (1)		18.08	133907	114
10	Chrysene (2)		18.21	992122	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 3: 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.

List of Figures

1 Naphtalene 4
2 Acenaphthene 4
3 Acenaphthylene 4
4 Fluorene 4
5 Phenanthrene 4
6 Anthracene 4
7 Chrysene 4
8 Fluoranthene 4
9 Pyrene 4

List of Tables

1 Diluted solution ratios 3
2 Compounds data 4

List of Equations

1 Stock solution volume 3
2 Solvent volume 3
3 Concentration of Chrysene in the unknown sample 5