

# TGA-IR

- Termogravimetrická analýza spojená s infračervenou spektrometrií

- Detekce úbytku hmotnosti v závislosti na teplotě –

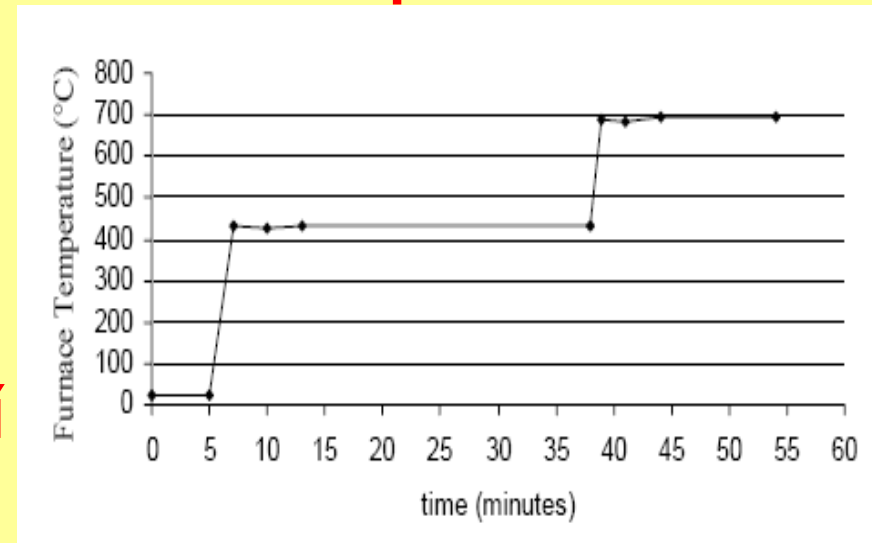
- Efekt rostoucí teploty
- Kinetika procesu
  - Lineárně rostoucí teplota ,  
isotermické úseky

- Fyzikální procesy – odpařování
- Chemické procesy – rozklad

- Studium léčiv

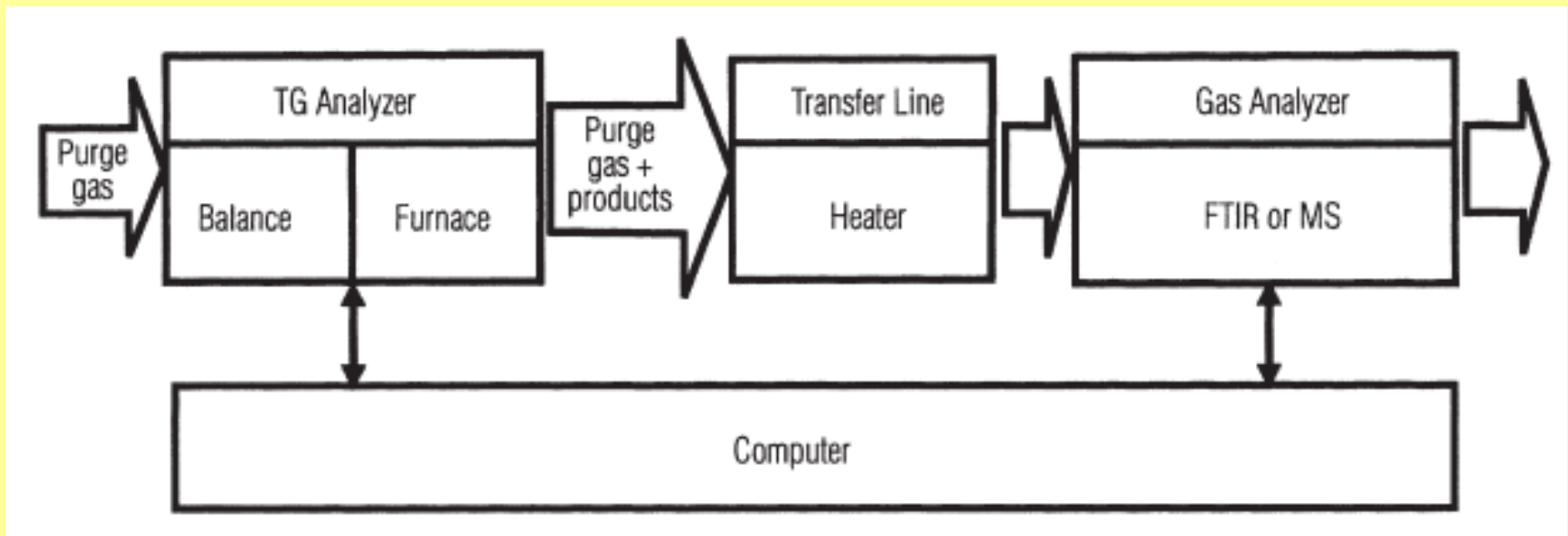
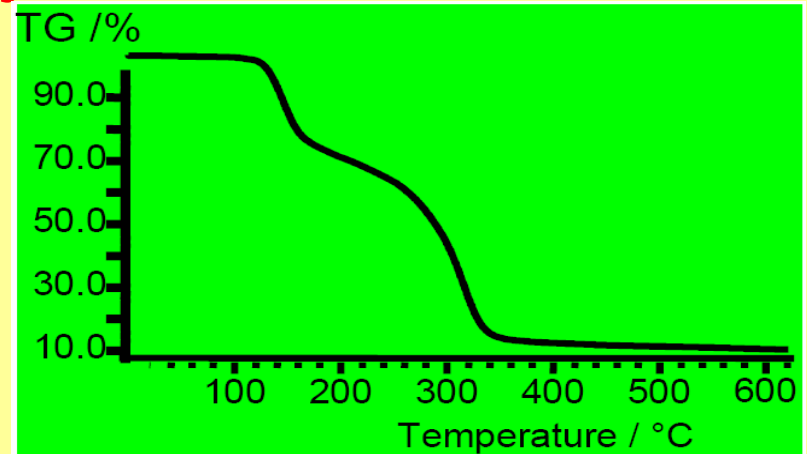
- Studium anorganických materiálů

- Studium polymerů – typické termodegradační chování jednotlivých polymerů



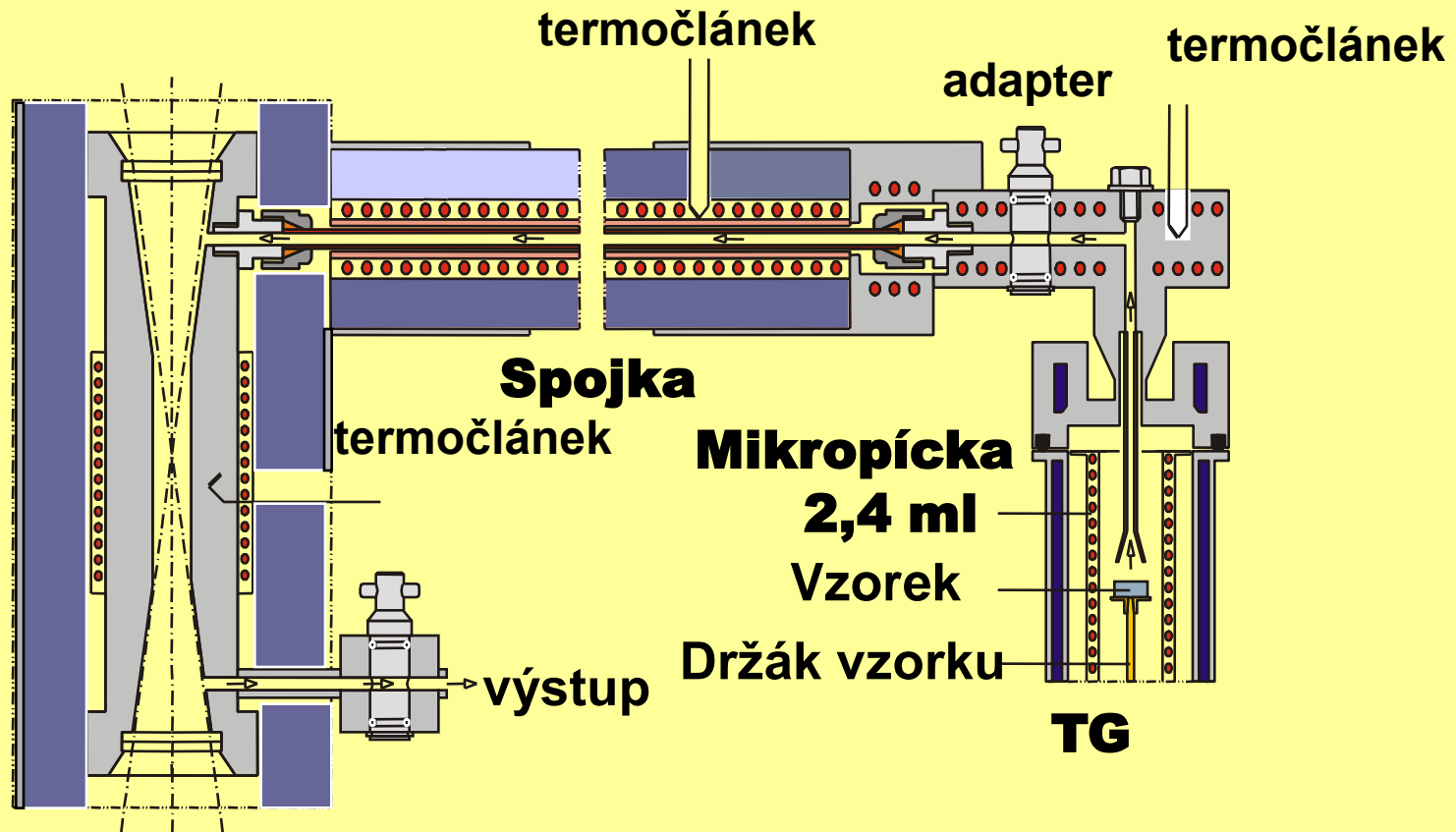
# TGA-IR

- Termogravimetrická analýza spojená s infračervenou spektrometrií
  - Detekce úbytku hmotnosti v závislosti na teplotě
  - Detekce těkavých produktů tepelného rozkladu IR spektrometrií



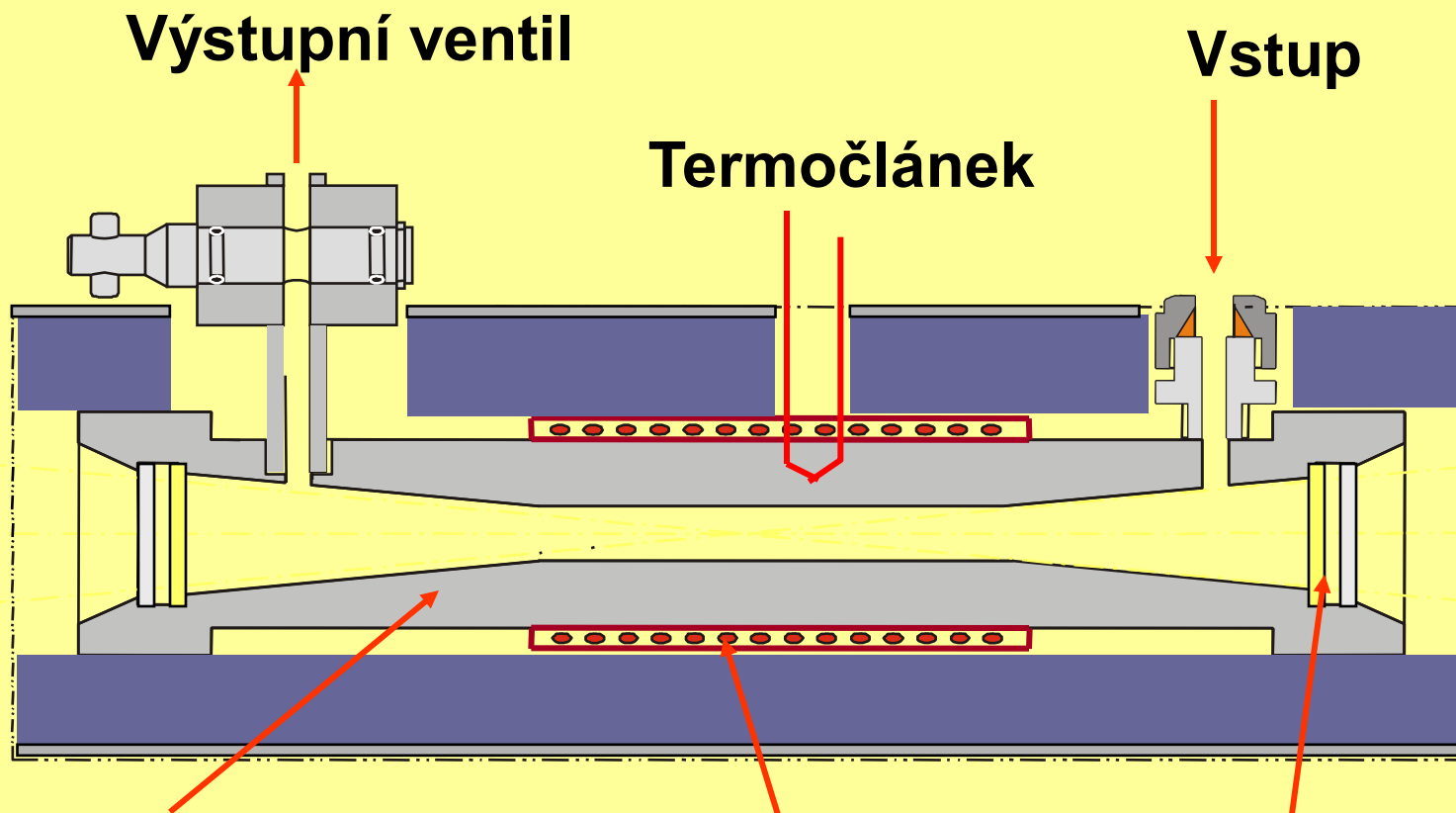
# TGA-IR

- Termogravimetrická analýza spojená s infračervenou spektrometrií - interface



# KONSTRUKCE PLYNOVÉ CELY

# TGA-IR



Ocelové pouzdro

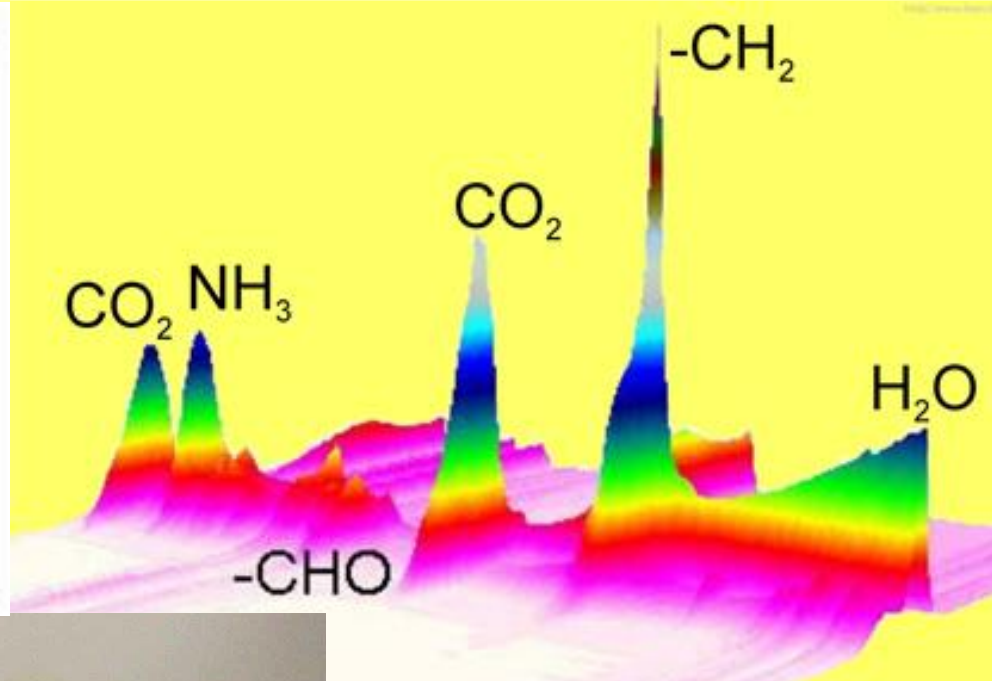
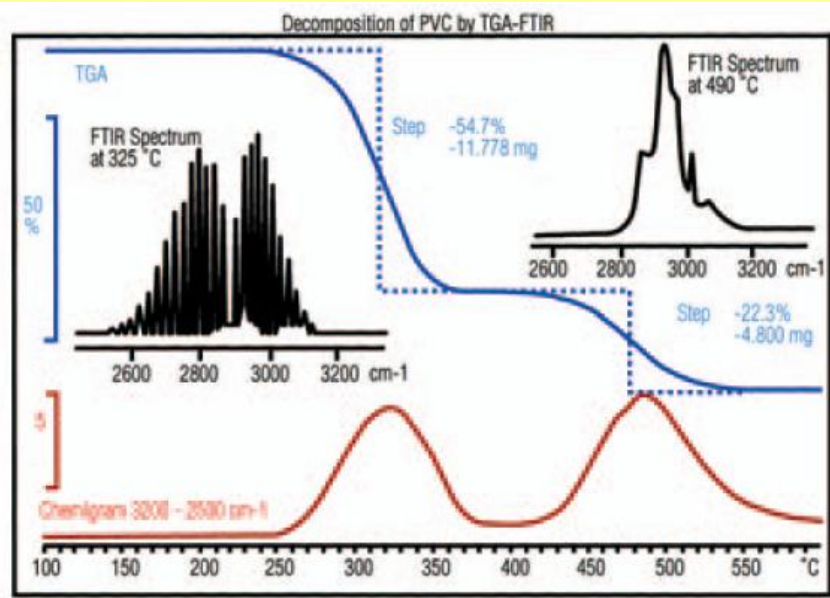
Ohříváč

Dvojitá okénka  
- KBr, ZnSe

**Objem cely: 8.7 ml**  
**Délka: 123 mm**

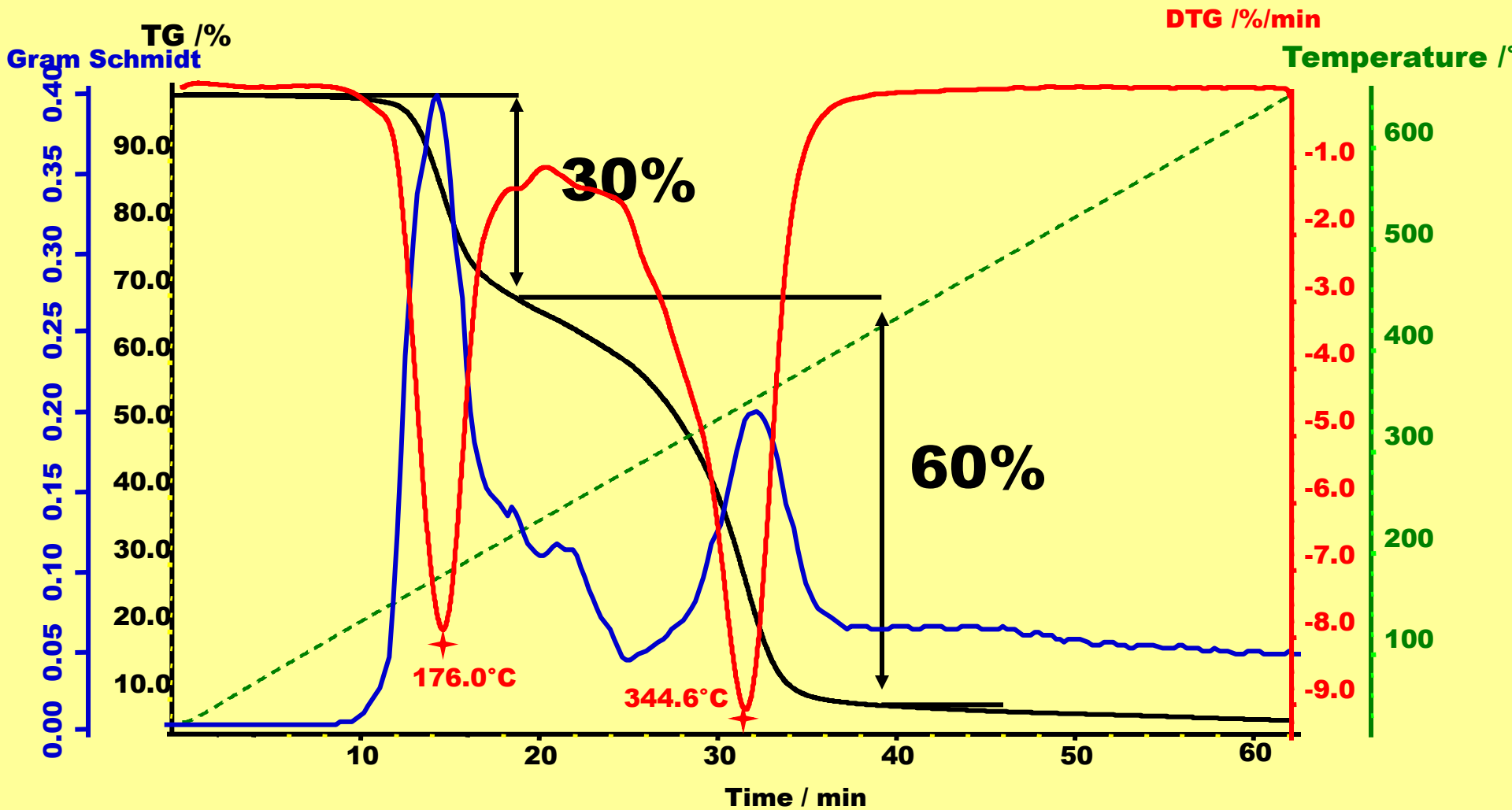
# TGA-IR

- Termogravimetrická analýza spojená s FTIR



# Aspirin<sup>®</sup>

# TGA-IR



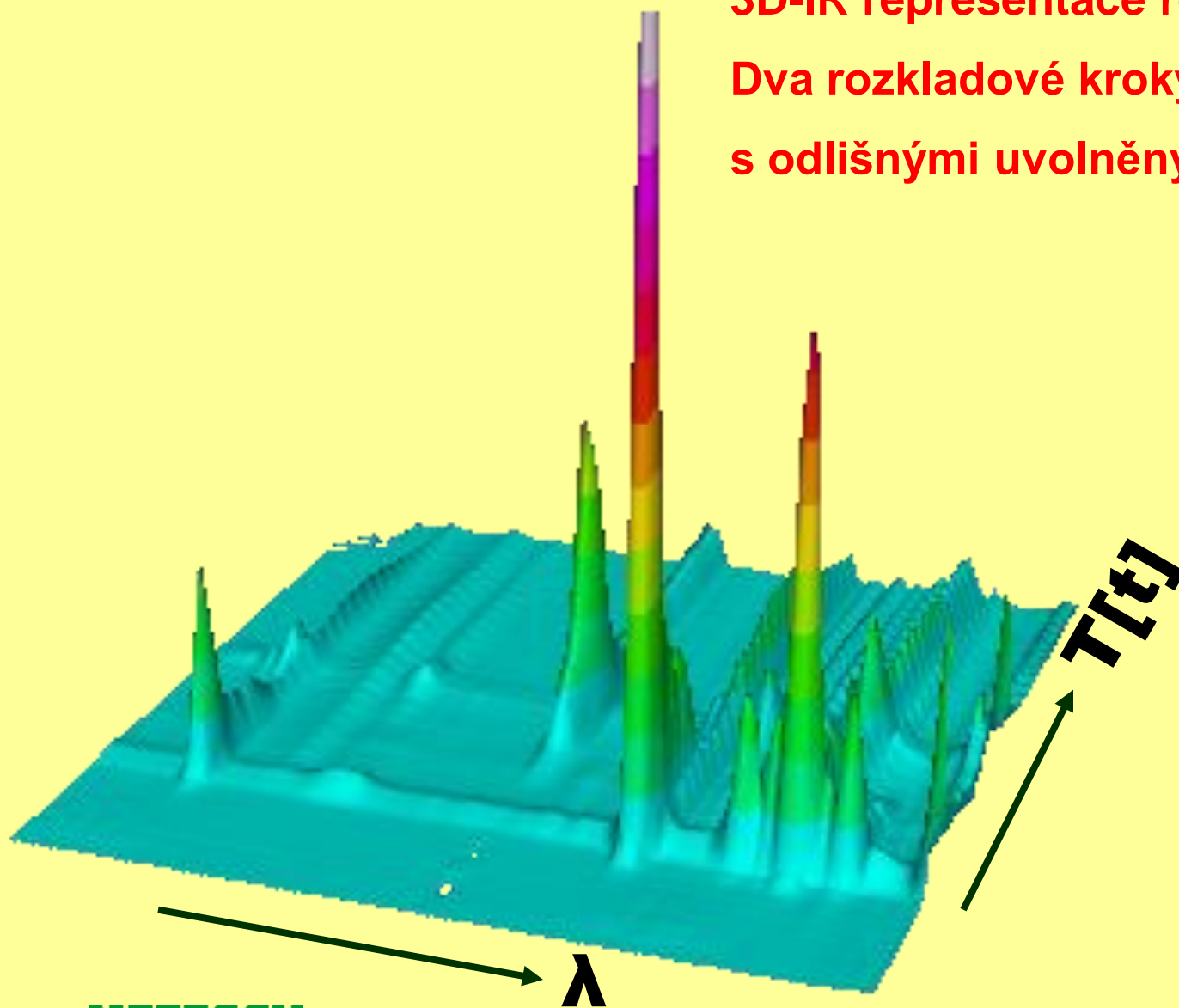
# TG/FT-IR Applications

ASPIRIN® 3-D VIEW

3D-IR representace rozkladu ASPIRINU.

Dva rozkladové kroky

s odlišnými uvolněnými plyny.

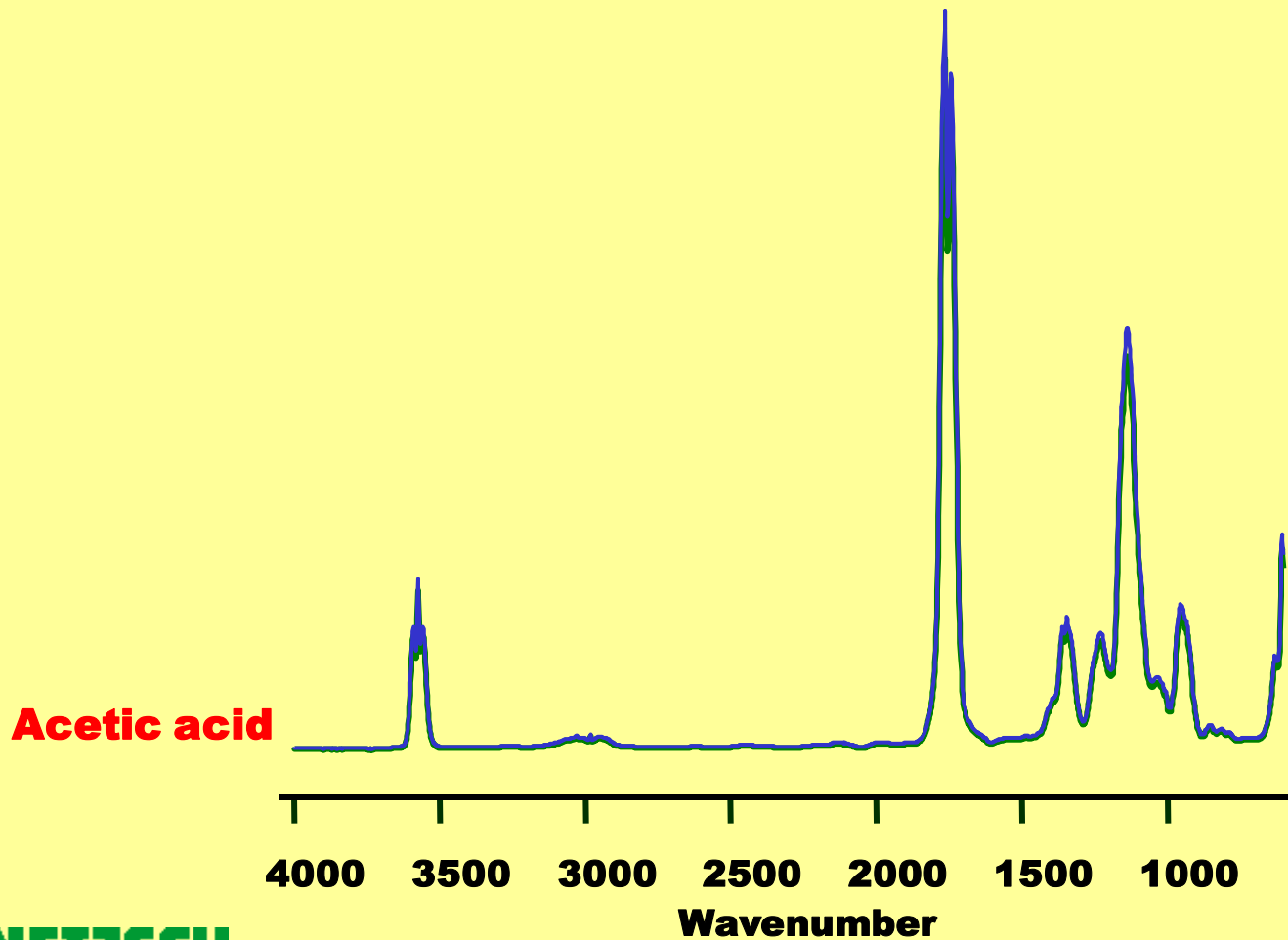


TG + FT-IR: More than Just the Sum of Its Parts

# TG/FT-IR Applications

## ASPIRIN® SPECTRUM OF EVOLVED GAS 175°C

Spectrum at the decomposition temperature of 175°C





# TG/FT-IR Applications

## ASPIRIN® LIBRARY SEARCH OF SPECTRUM RELEATED TO 175°C

The screenshot displays the OPUS software interface. The main window shows an FT-IR spectrum with two traces (red and blue) plotted against wavenumber from 4000 to 500 cm⁻¹. The y-axis represents intensity from 0.00 to 1.00. A prominent peak is visible at approximately 1710 cm⁻¹. Below the spectrum, a search results table is shown:

Hit No.	Hit Qual.	Compound Name
1.	695	ACETIC ACID
2.	560	VANILLIN ACETATE

Below the table, a 'Substanzinformation' (Substance Information) panel is visible, providing details for Acetic Acid:

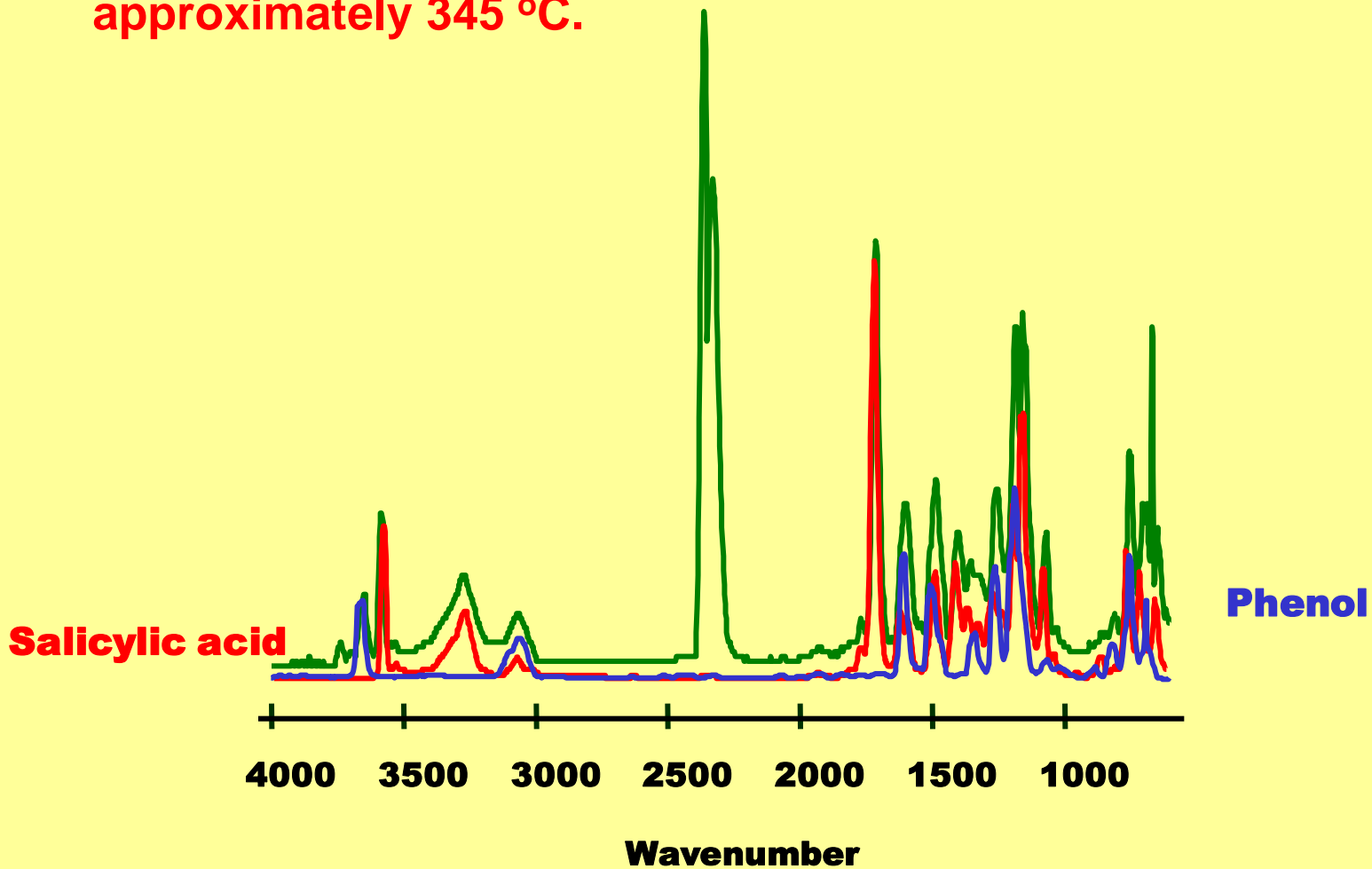
Substanzinformation	
Compound Name	ACETIC ACID
Molecular Formula	C2H4O2
Molecular Weight	60.05
CAS Registry Number	64-19-7
Sadtler ID-Number	EL00504
Melting Point	16.2C
Boiling Point	118C

The interface also includes a file explorer on the left, a menu bar with options like 'Datei', 'Bearbeiten', and 'Anzeige', and a taskbar at the bottom showing the Start button and open applications like OPUS and Microsoft PowerPoint.

# TG/FT-IR Applications

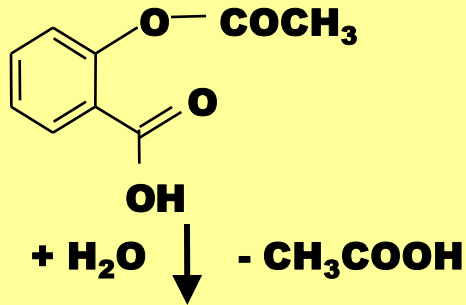
ASPIRIN®

Extracted spectra at a decomposition temperature of approximately 345 °C.

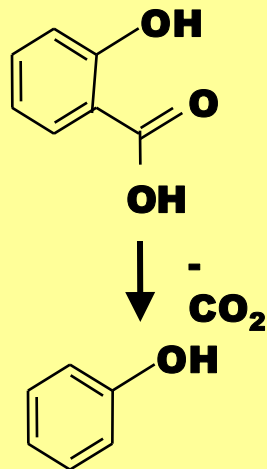


# TG/FT-IR Applications

ASPIRIN® TYPICAL OPUS SEARCH VIEW



**Acetyl Salicylic Acid**  
**(Aspirin®)**



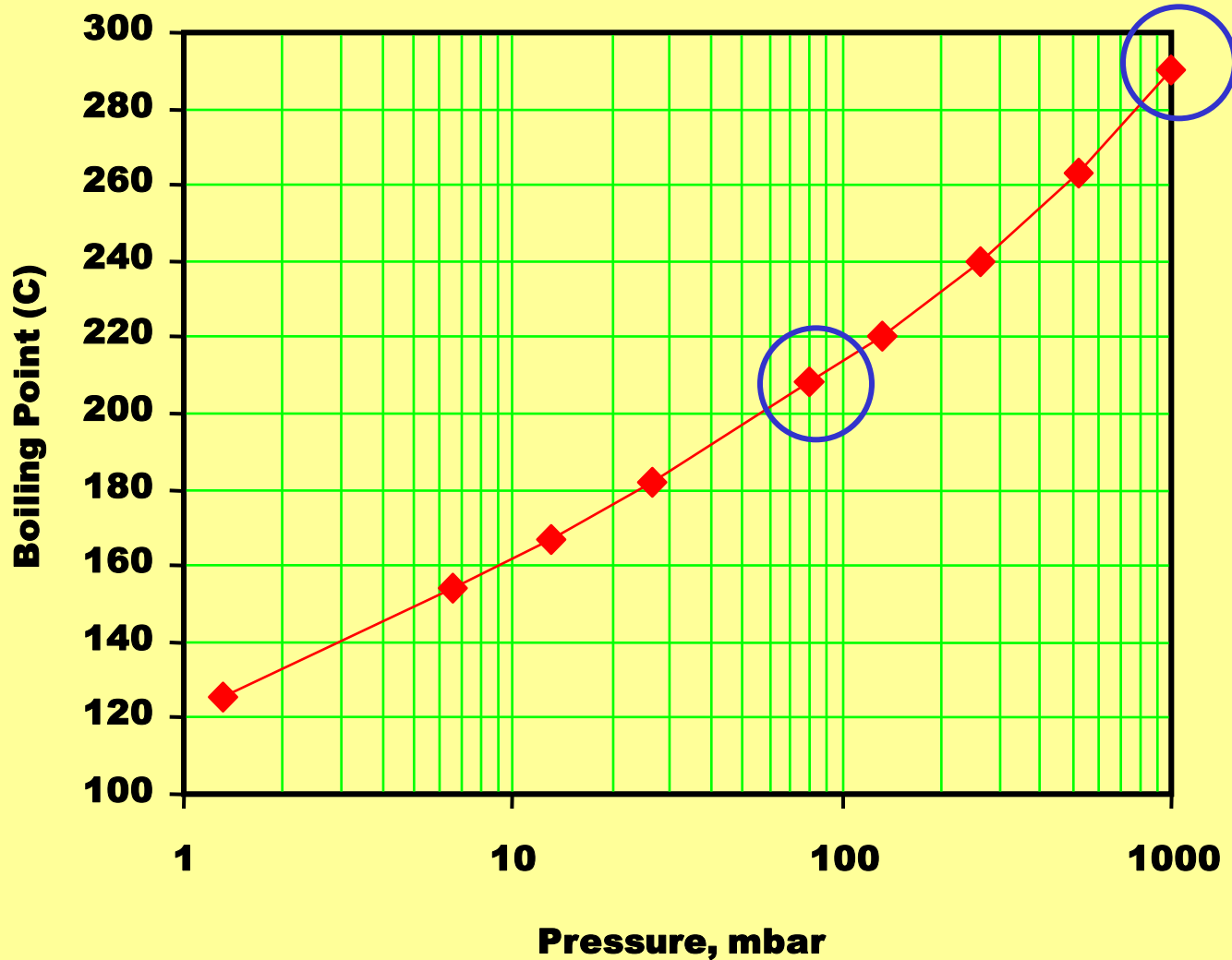
**Salicylic Acid**

**bp. at 1013 mbar, 211°C**

**Phenol**

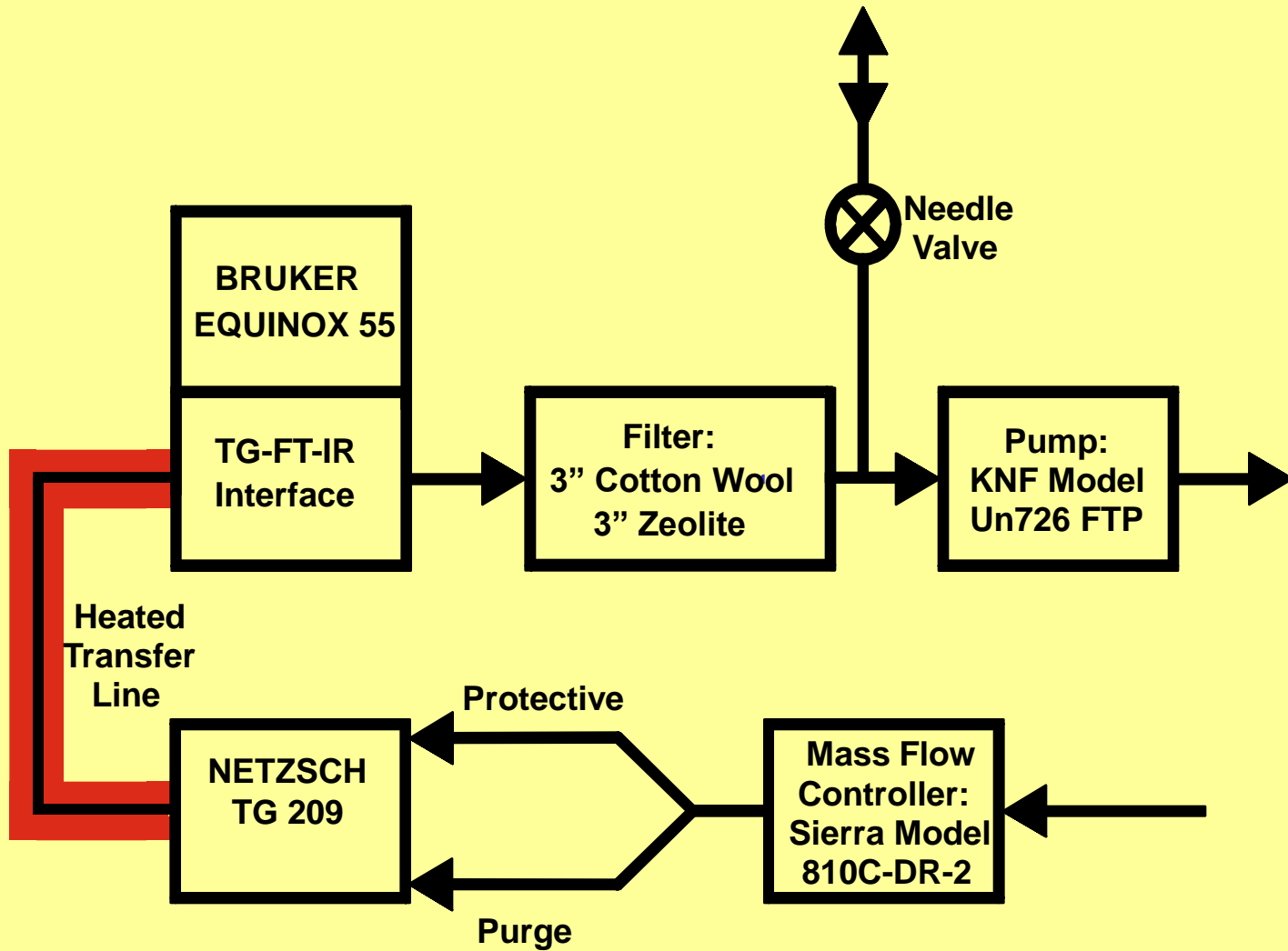
**bp. at 1013 mbar, 181°C**

# Glycerol: Boiling Point as a Function of Pressure



# Reduced Pressure TG/FT-IR

## EXPERIMENTAL SETUP

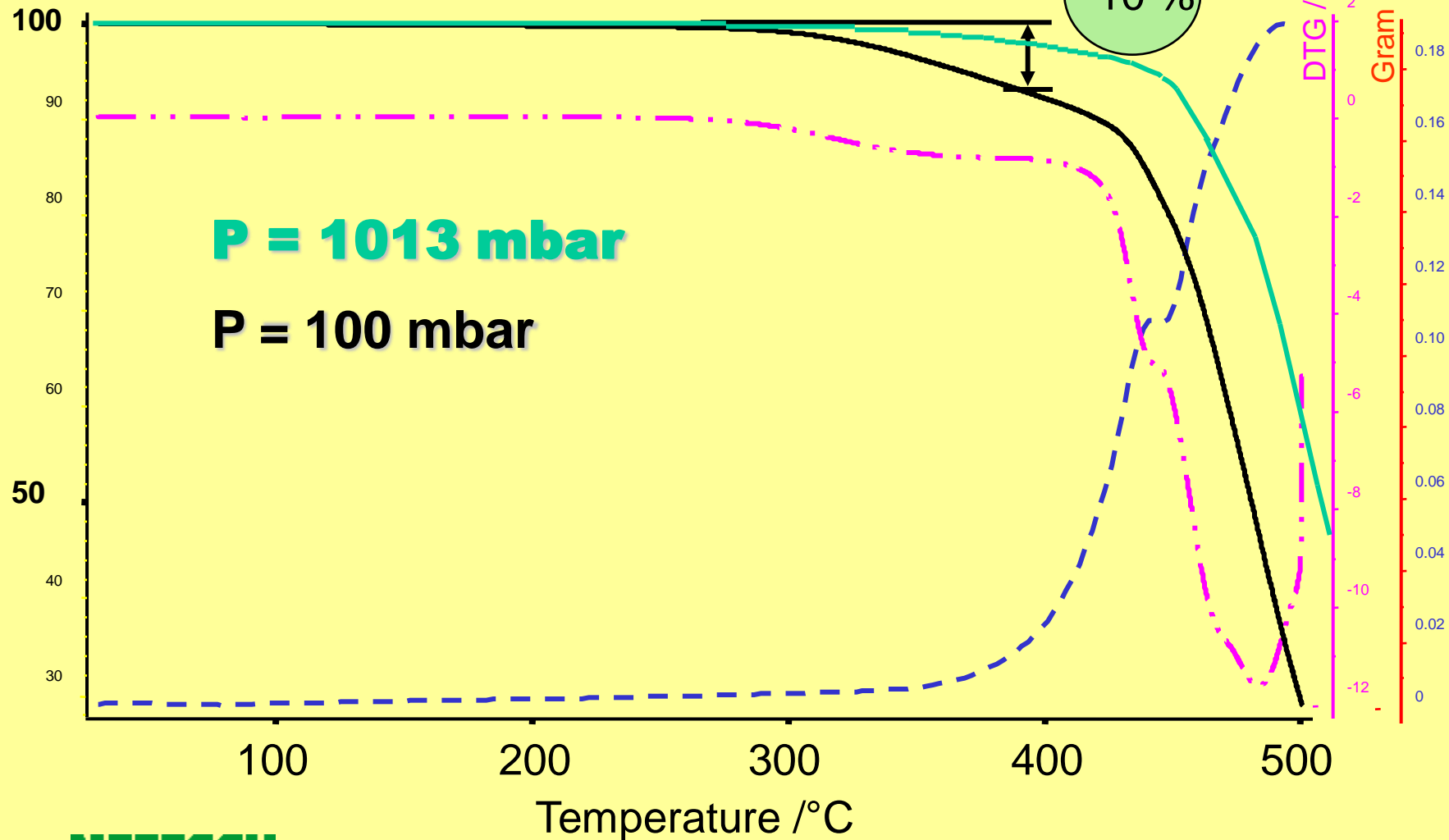


TG + FT-IR: More than Just the Sum of Its Parts

# TG/FT-IR Applications

PERFLUORATED ELASTOMER

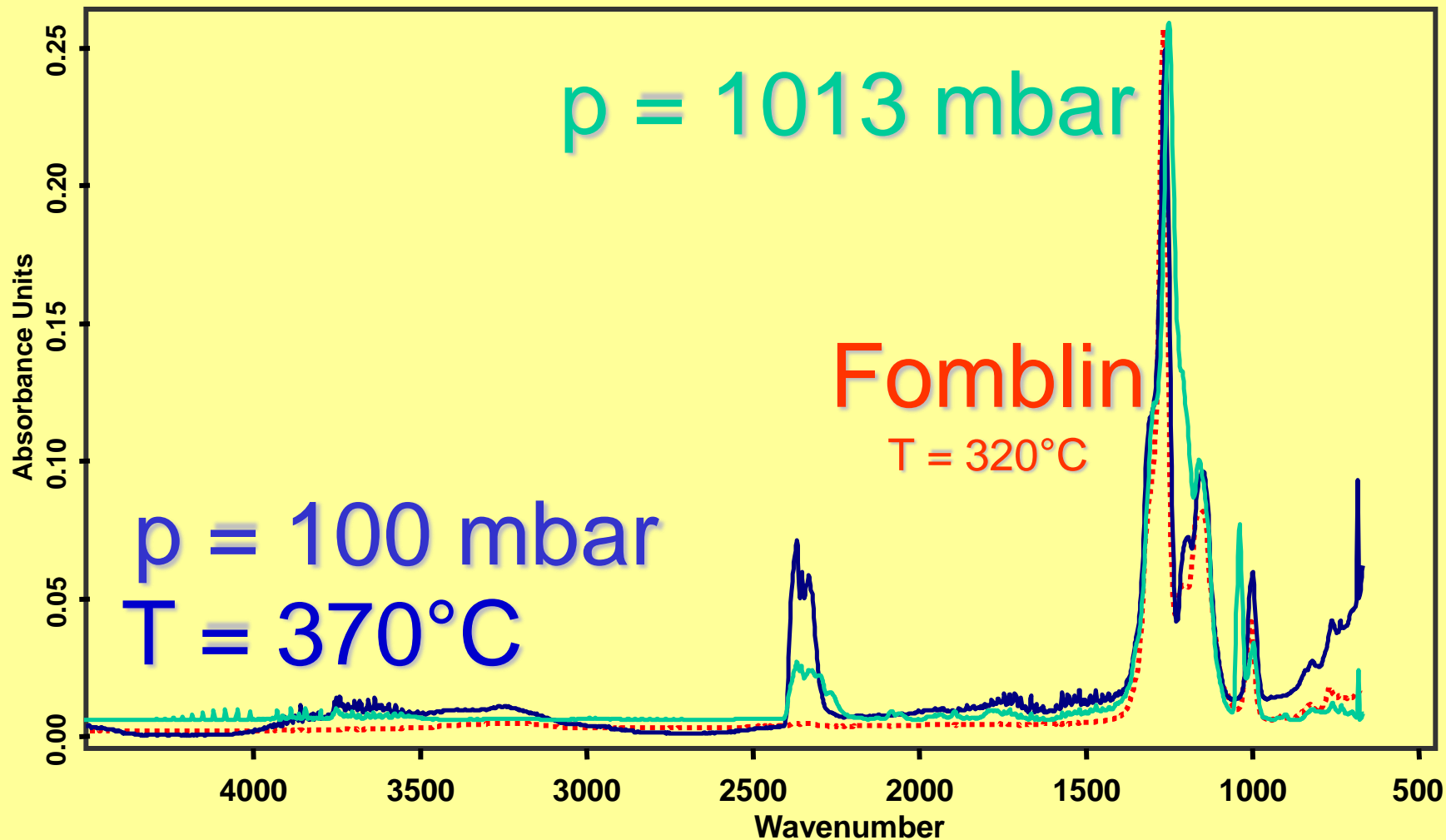
TG /%



TG + FT-IR: More than Just the Sum of Its Parts

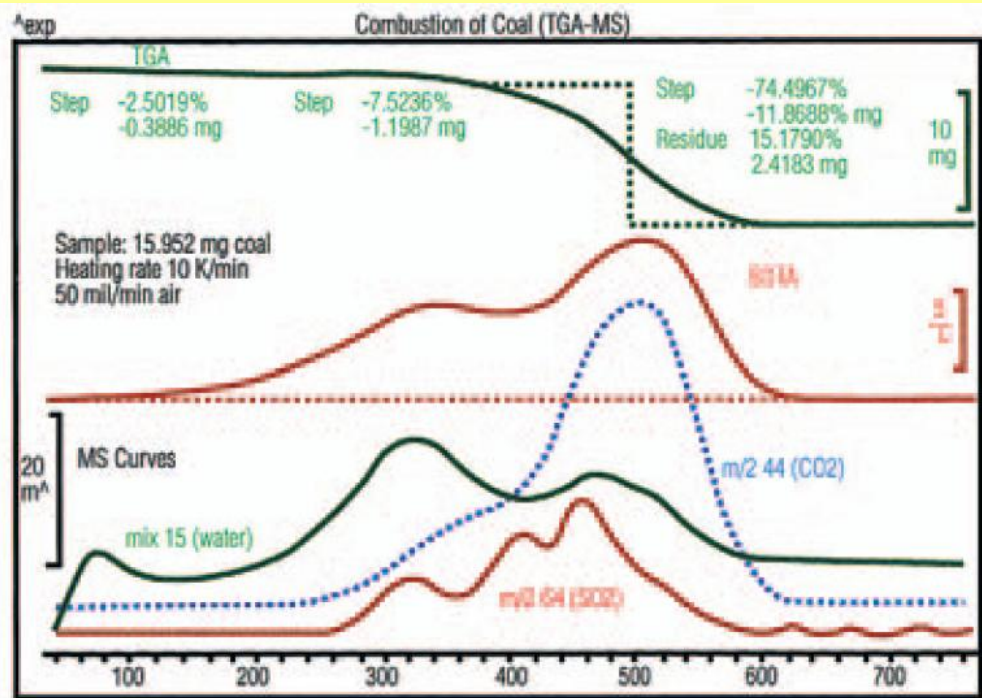
# TG/FT-IR Applications

PERFLUORATED COMPOUNDS: SOFTENER

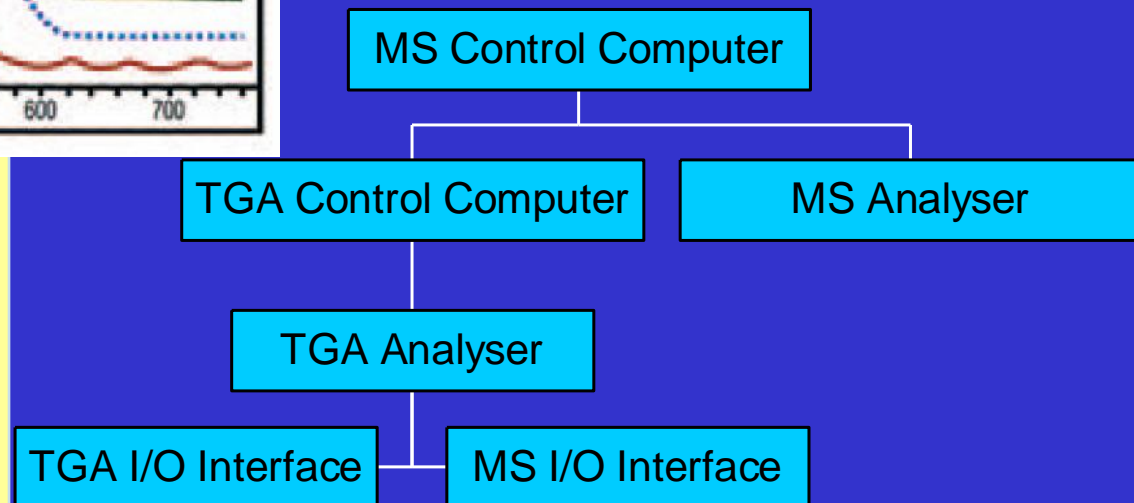


# TGA-MS

- Termogravimetrická analýza spojená s MS spektrometrií
  - Detekce těkavých produktů tepelného rozkladu MS

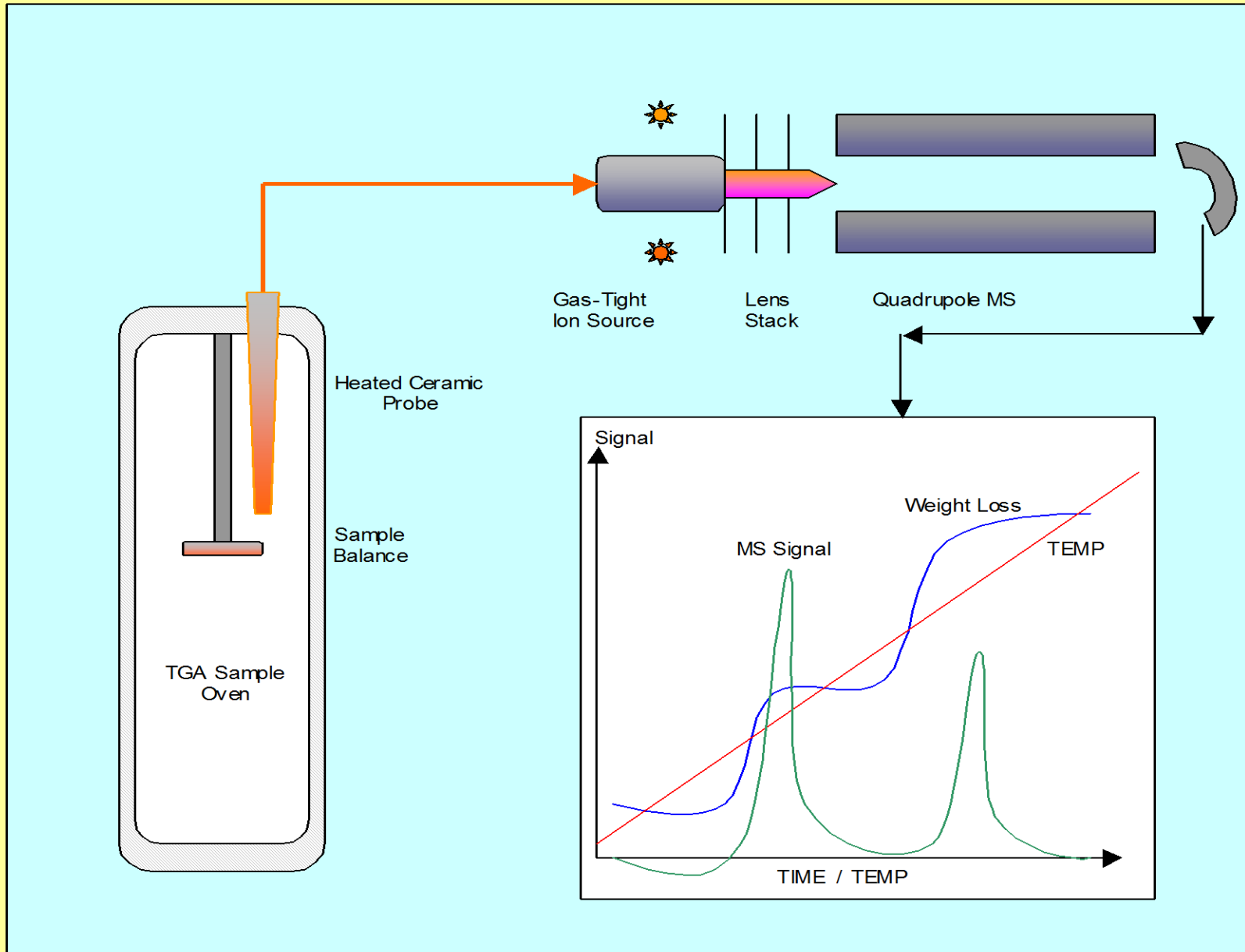


TGA-MS Link Technique  
Analogue / Digital Interfacing

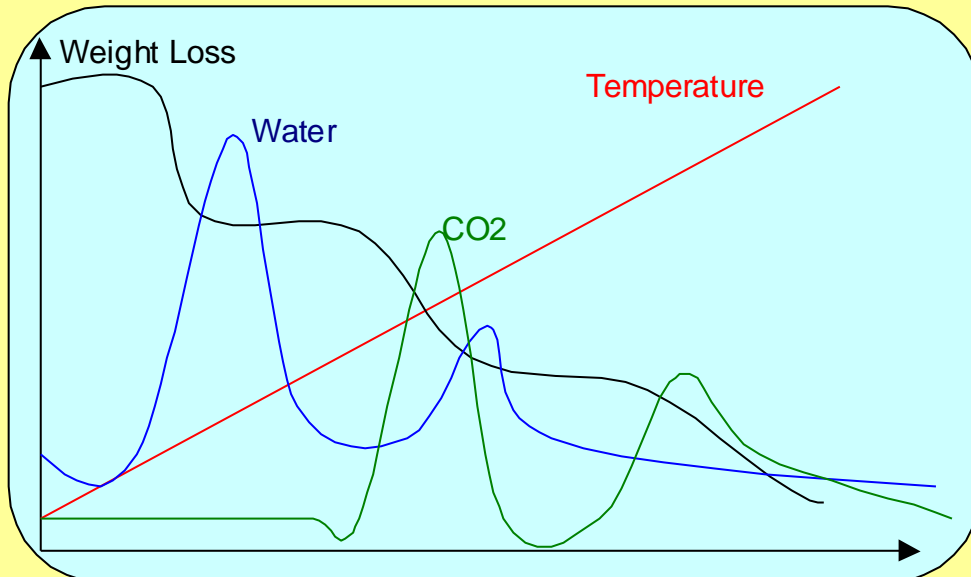




# TGA-MS - schéma



# TGA-MS



➤ **Ztráty hmotnosti**

➤ **MS křivky**

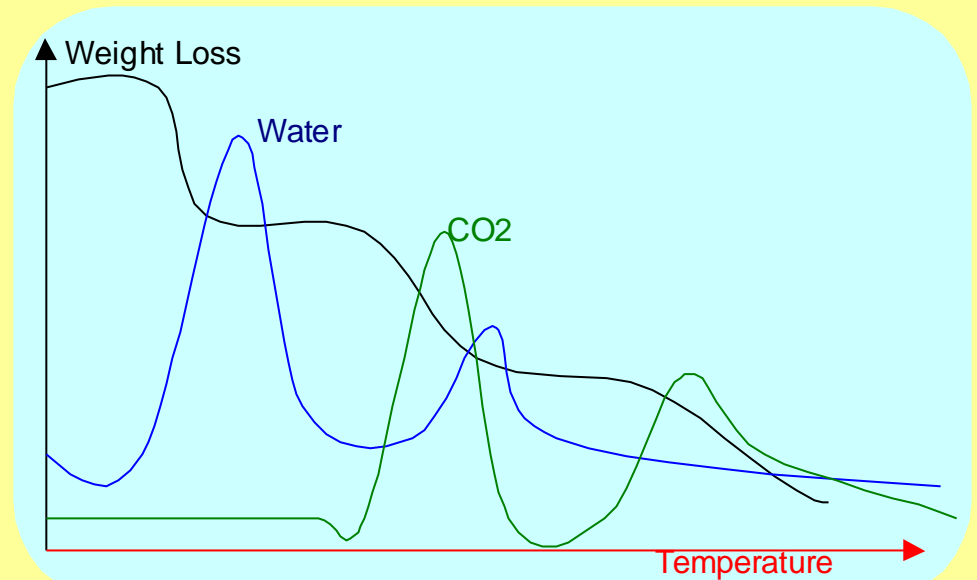
➤ **Teplotní záznam**

**vůči času**

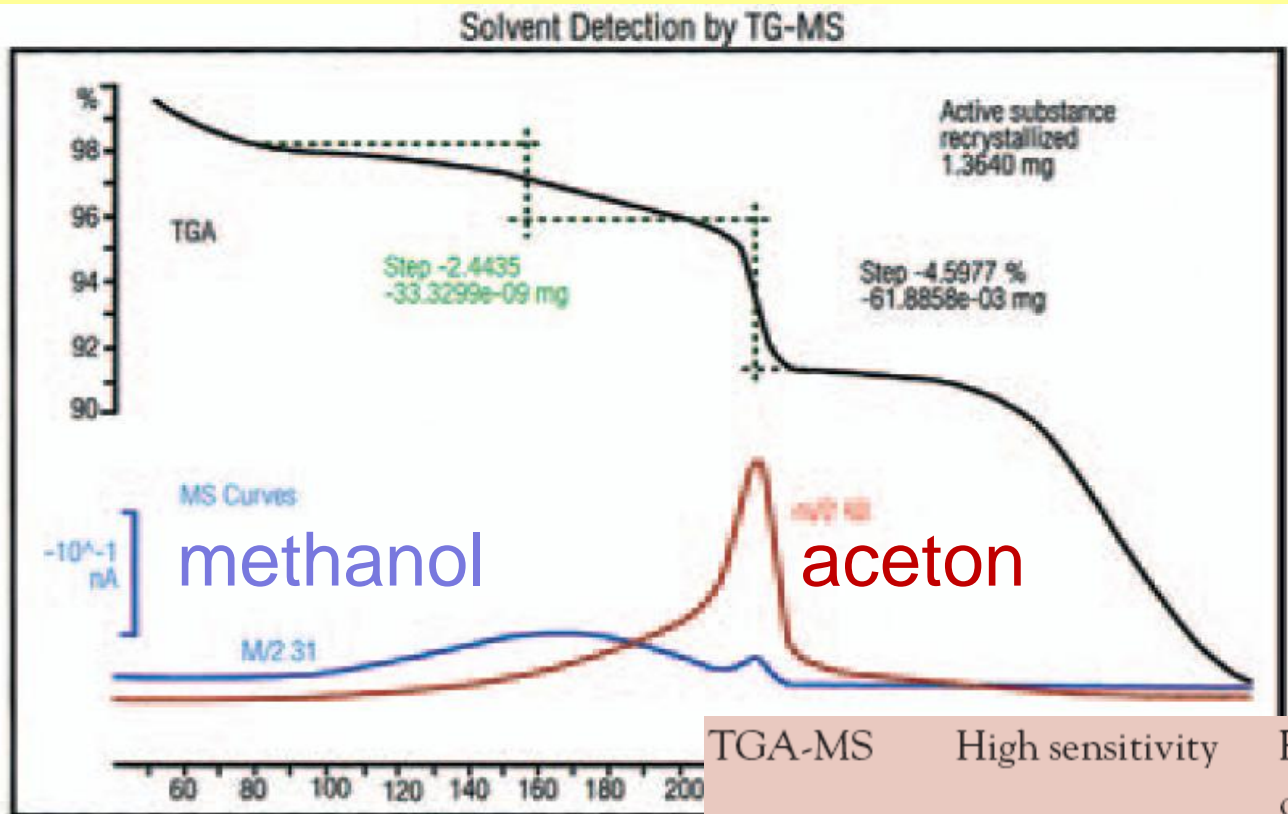
➤ **Ztráty hmotnosti**

➤ **MS křivky**

**vůči teplotě**



# TGA-MS



TGA-MS

High sensitivity

Extremely low concentrations of evolved gases can still be identified (e.g., impurities in pharmaceutical substances)

High resolution (time scale)

Overlapping weight losses can be interpreted qualitatively

TGA-FTIR

High chemical specificity

Direct identification of compounds and functional groups

High resolution (time scale)

Overlapping weight losses can be interpreted quantitatively