



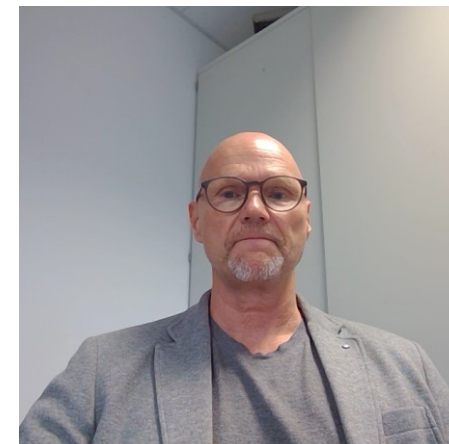
# SNIF-NMR Analysis of Wine

Carsten Fauhl-Hassek

# SNIF-NMR<sup>®</sup>

## Site-specific Natural Isotope Fractionation-Nuclear Magnetic Resonance

- **What is it ?**
  - Quantitative <sup>2</sup>H-NMR + calculation
- **What do we obtain ?**
  - Delivers the deuterium content at different sites of a molecule
- **Why is it of interest ?**
  - The deuterium pattern is found to be highly discriminating between natural and synthetic compounds

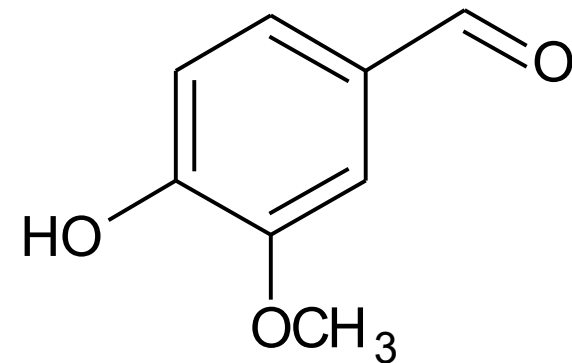
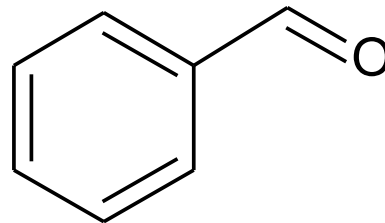
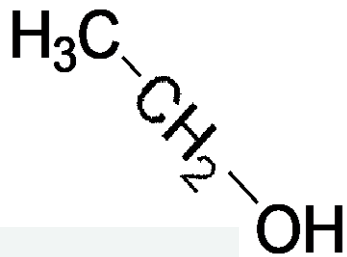


# SNIF-NMR®



Widely used for authentication

- Wine, fruit juice and flavours: benzaldehyde, vanillin etc.
- e.g. aldehyde groups often highly enriched in synthetic compounds





## Advantages

- Highly discriminating, provides botanical and geographical information
- In some cases the only possibility of proof of authenticity
- Almost impossible to manipulate the deuterium pattern

## Disadvantages

- Expensive and time consuming
- Applicable only to pure substances, > 150 mg
- Extensive isolation procedures necessary, often preparative HPLC

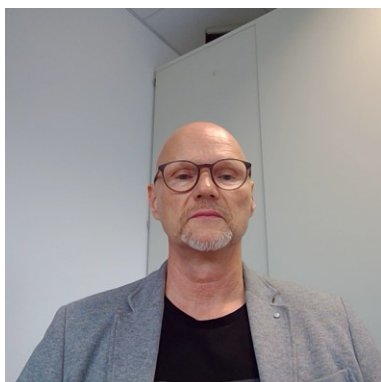
# International Organisation of Vine and Wine

[www.oiv.com](http://www.oiv.com)  
**Compendium of Int. Methods of  
Anal.**

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**COMPENDIUM OF  
INTERNATIONAL METHODS  
OF WINE AND MUST ANALYSIS**

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INTERNATIONAL ORGANISATION  
OF VINE AND WINE

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**COMPENDIUM OF INTERNATIONAL METHODS OF ANALYSIS-OIV**  
**Table of contents**

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General organization of the Compendium

Table of contents

Foreword

**ANNEX A – METHODS OF ANALYSIS OF WINES AND MUSTS**

**SECTION 1 – DEFINITIONS AND GENERAL PRINCIPLES**

**SECTION 2 – PHYSICAL ANALYSIS**

**SECTION 3 – CHIMICAL ANALYSIS**

**SECTION 3.1 – ORGANIC COMPOUNDS**

*SECTION 3.1.1 – SUGARS*

*SECTION 3.1.2 – ALCOHOLS*

*SECTION 3.1.3 – ACIDS*

*SECTION 3.1.4 – GAS*

*SECTION 3.1.5 – OTHER ORGANIC COMPOUNDS*

**SECTION 3.2 – NON ORGANIC COMPOUNDS**

*SECTION 3.2.1 – ANIONS*

*SECTION 3.2.2 – CATIONS*

*SECTION 3.2.3 – OTHER NON ORGANIC COMPOUNDS*

**SECTION 4 – MICROBIOLOGICAL ANALYSIS**

**SECTION 5 – OTHER ANALYSIS**

**ANNEX B - CERTIFICATES OF ANALYSIS**

**ANNEX C - MAXIMUM ACCEPTABLE LIMITS OF VARIOUS SUBSTANCES**

**ANNEX D – ADVICES**

**ANNEX E – LABORATORY QUALITY ASSURANCE**

**ANNEX F – SPECIFIC METHODS FOR THE ANALYSIS OF GRAPE SUGAR  
(RECTIFIED CONCENTRATED MUSTS)**

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OIV-MA-INT-00-2018

1

# Techniques for Stable Isotope Analysis

- Site-Specific Natural Isotope Fractionation-Nuclear Magnetic Resonance spectroscopy (**SNIF-NMR**)
  - site-specific analysis within one molecule

**D/H of  
wine ethanol**

COMPENDIUM OF INTERNATIONAL ANALYSIS OF METHODS - OIV  
Determination of the deuterium distribution in ethanol by  
SNIF-NMR

Method OIV-MA-AS311-05

Type II method

- Isotope Ratio Mass Spectrometry (IRMS)
  - analysis of “bulk material” or separated compounds

**$^{13}\text{C}/^{12}\text{C}$  of  
wine ethanol**

COMPENDIUM OF INTERNATIONAL METHODS OF ANALYSIS - OIV  
Ethanol

Method OIV-MA-AS312-06

Type II method

**$^{18}\text{O}/^{16}\text{O}$  of  
wine water**

COMPENDIUM OF INTERNATIONAL METHODS OF ANALYSIS - OIV  
Isotopic ratio of water

Method OIV-MA-AS2-12

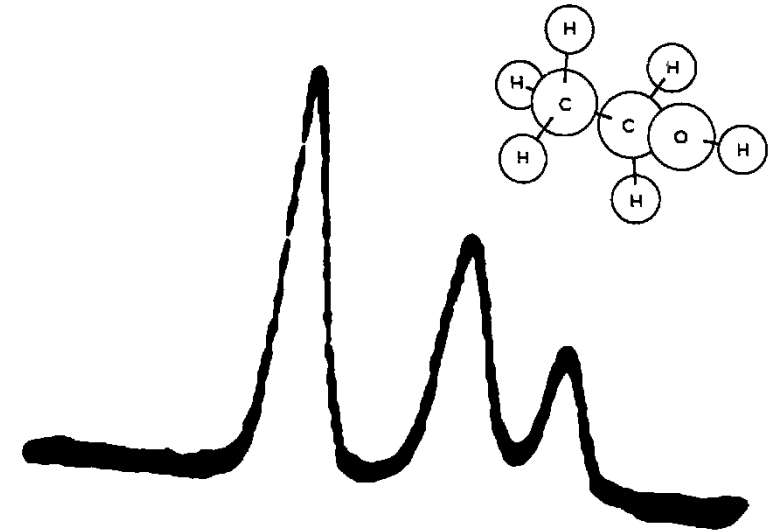
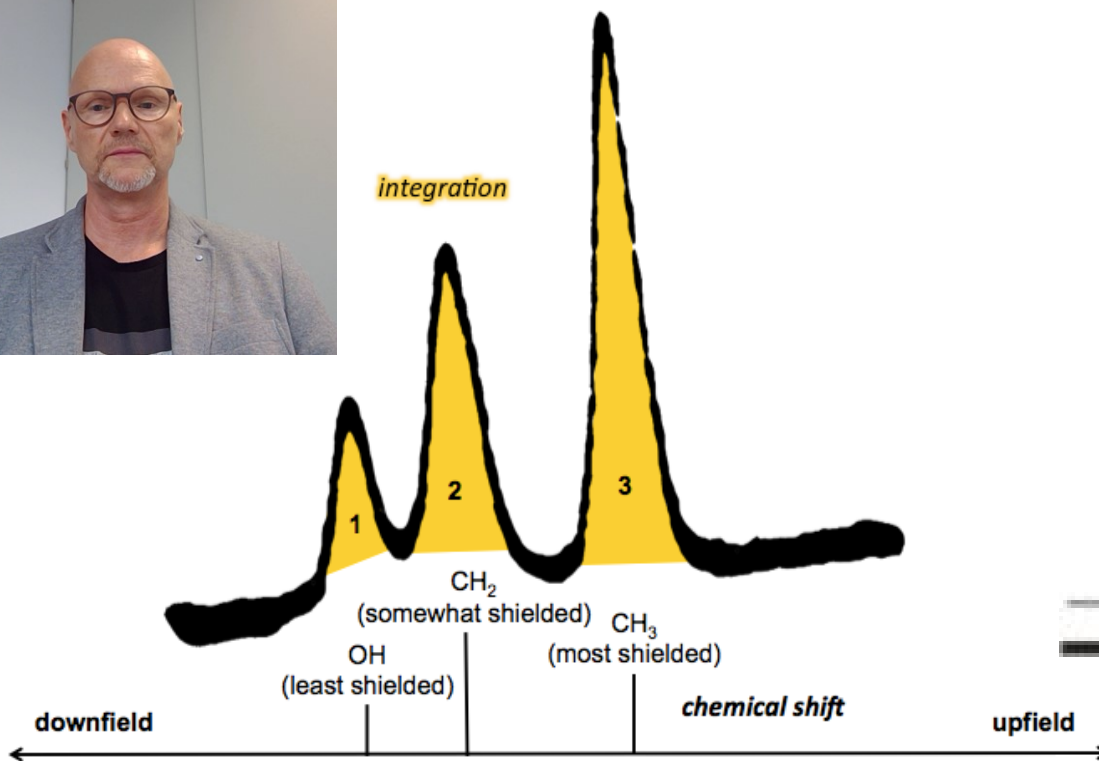
Type II method



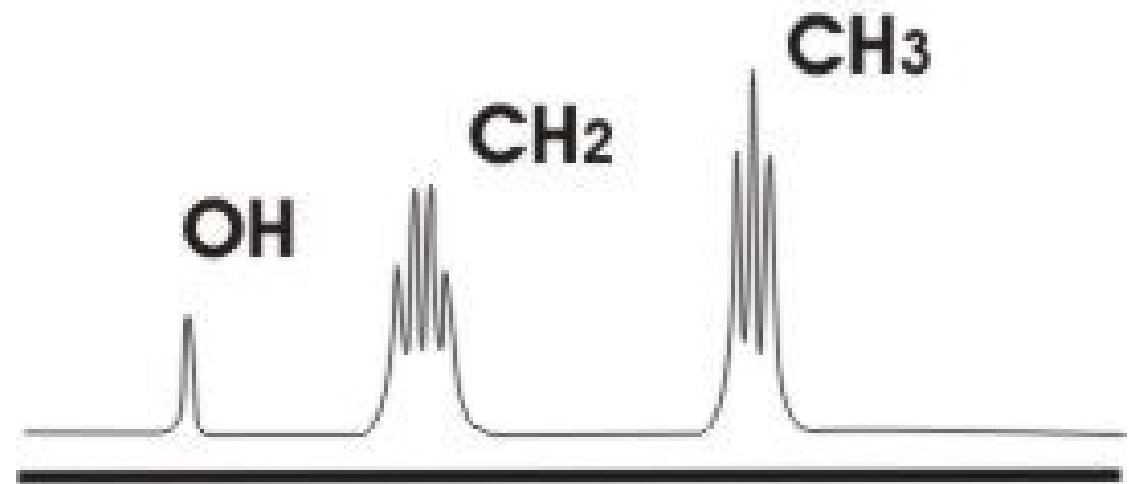


# NMR

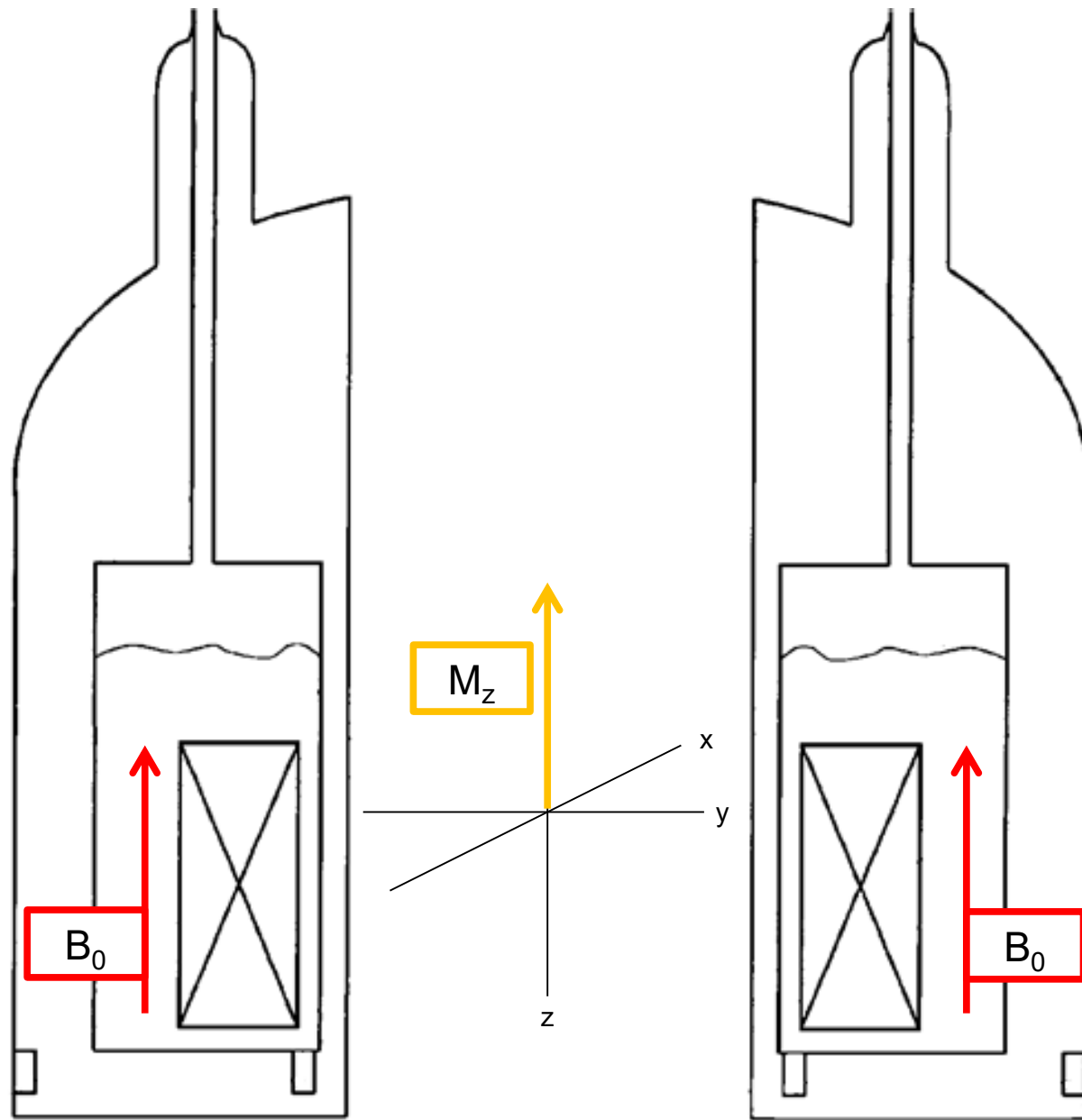
- Discovery of nuclear magnetic resonance by Edward Mills Purcell and Felix Bloch, Nobel price 1952



Early NMR-spectrum of ethanol (1951)  
(source: [www.wikipedia.org](http://www.wikipedia.org))

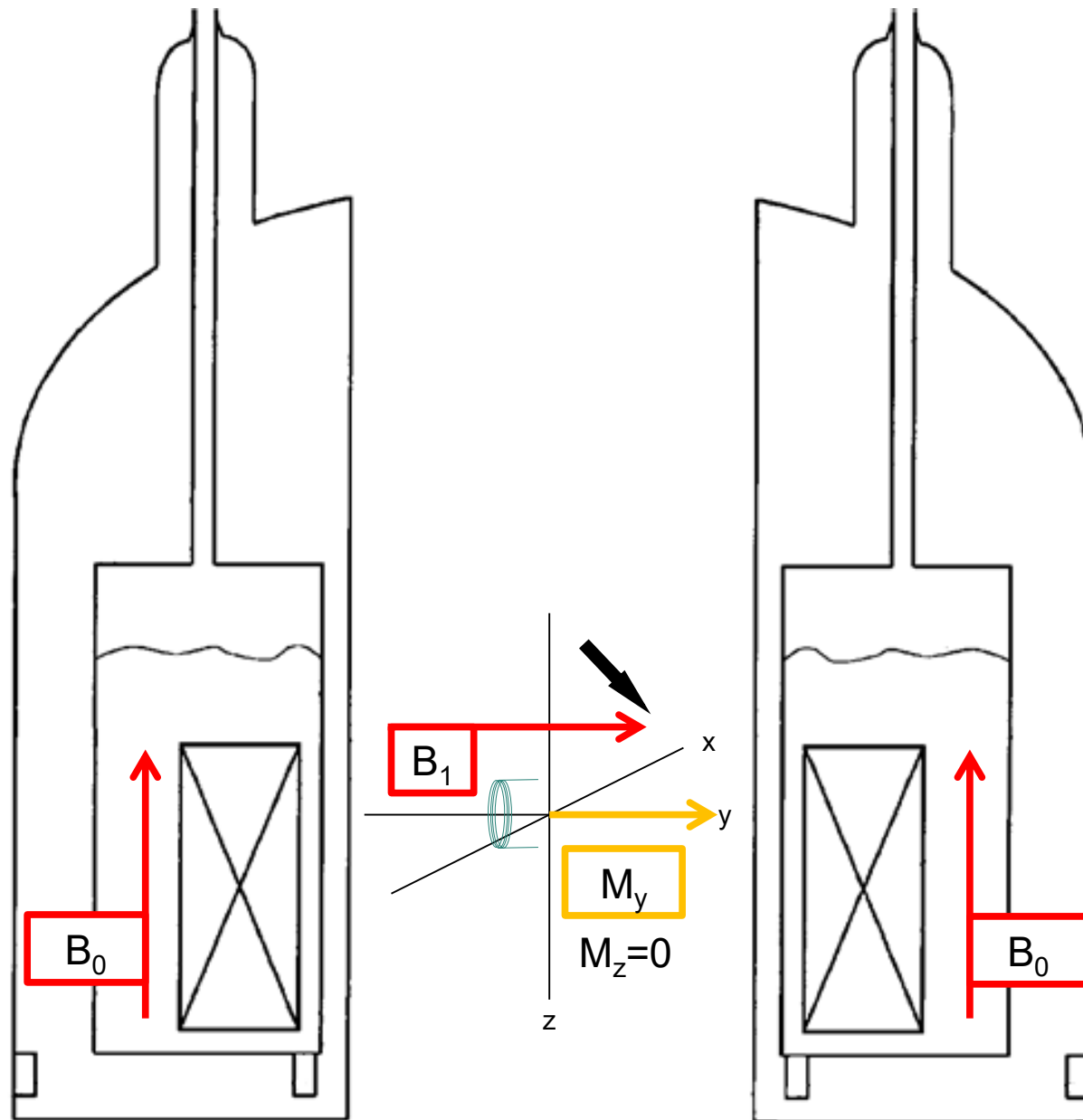


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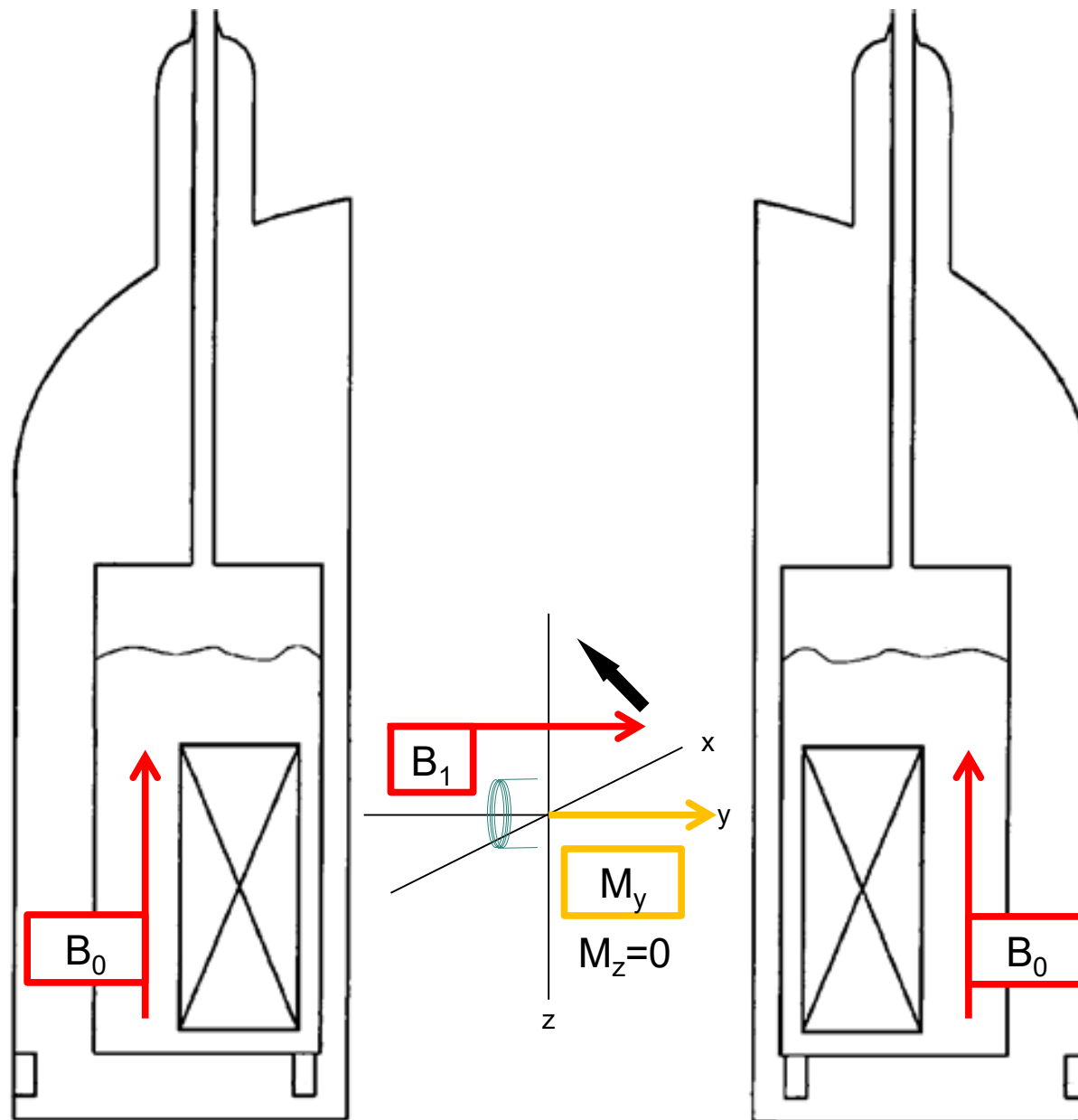
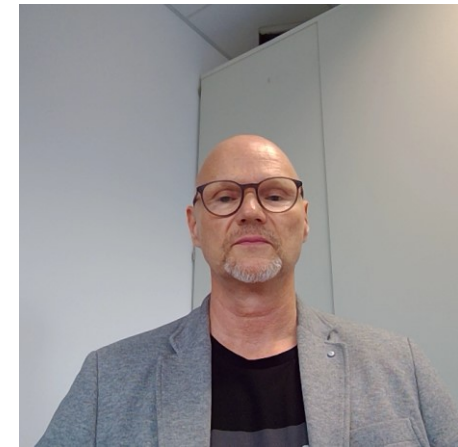




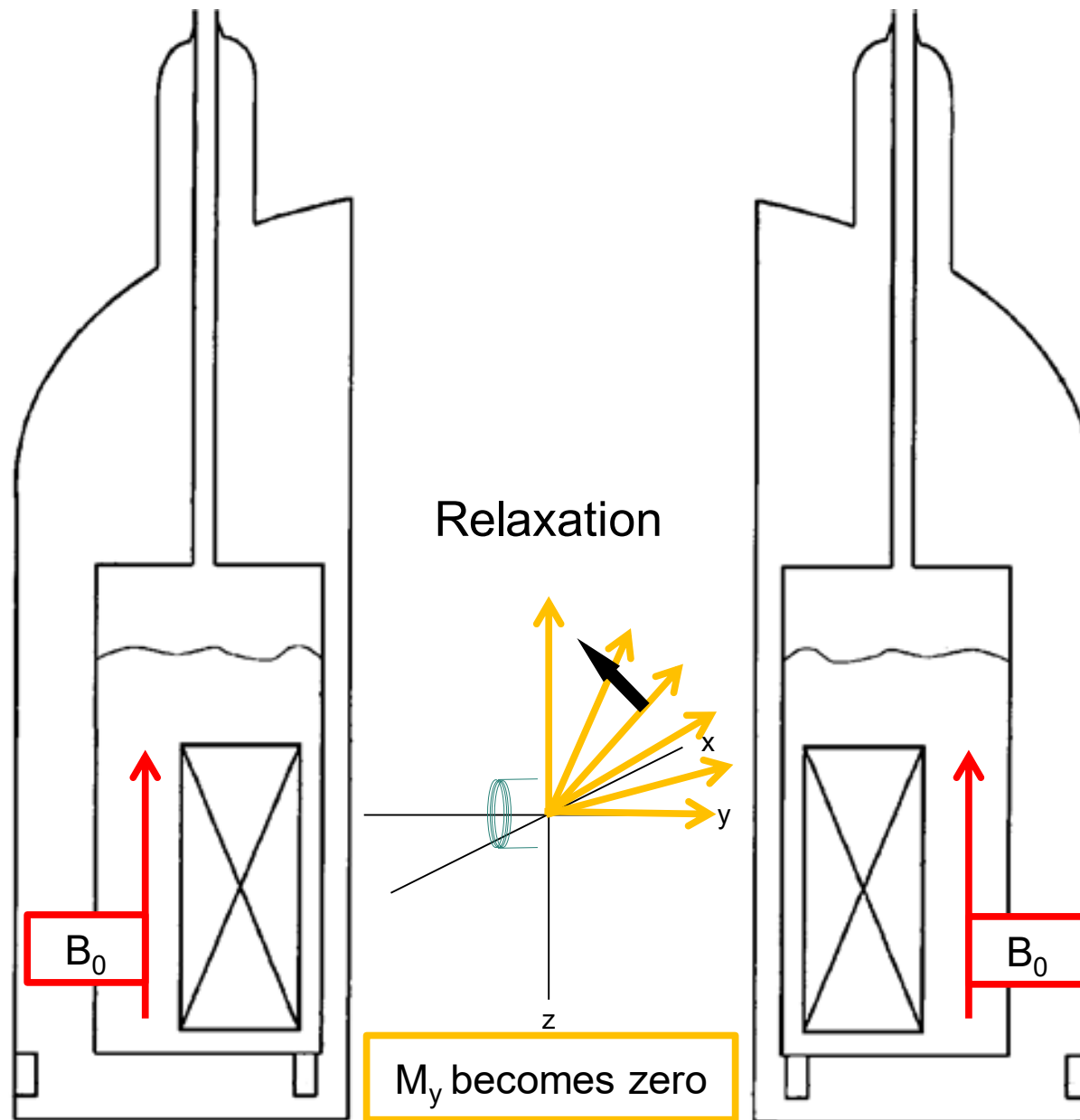
# NMR



# NMR



# NMR



## END Part A