GERMAN FEDERAL INSTITUTE
FOR RISK ASSESSMENT

BfR
Bundesinstitut für Risikobewertung

SNIF-NMR Analysis of Wine

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SNIF-NMR®

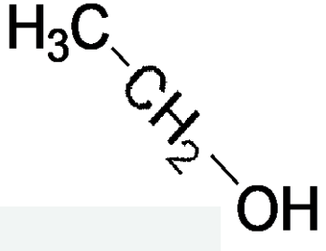
Site-specific **N**atural **I**sotope **F**ractionation-**N**uclear **M**agnetic **R**esonance

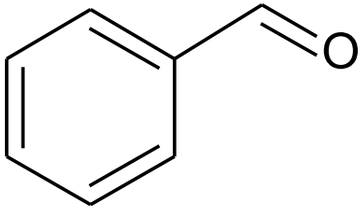
- **What is it ?**
  - Quantitative ^{2}H-NMR + calculation
- **What do we obtain ?**
  - Delivers the deuterium content at different sites of a molecule
- **Why is it of interest ?**
  - The deuterium pattern is found to be highly discriminating between natural and synthetic compounds

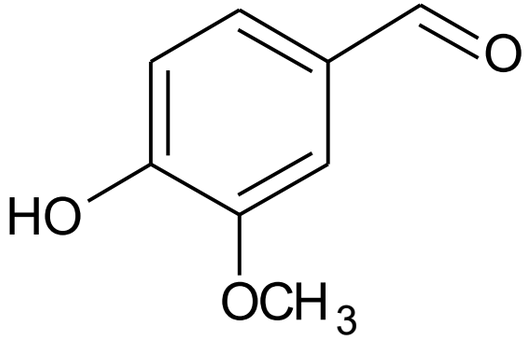
SNIF-NMR®

Widely used for authentication

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







SNIF-NMR®

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

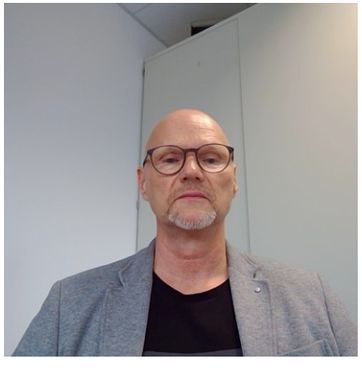
Disadvantages

- 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
Compendium of Int. Methods of Anal.

COMPENDIUM OF INTERNATIONAL METHODS OF WINE AND MUST ANALYSIS



OIV

INTERNATIONAL ORGANISATION OF VINE AND WINE

COMPENDIUM OF INTERNATIONAL METHODS OF ANALYSIS-OIV
Table of contents

General organization of the Compendium

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

$^{13}C/^{12}C$ of wine ethanol

COMPENDIUM OF INTERNATIOAL METHODS OF ANALYSIS - OIV
Ethanol

Method OIV-MA-AS312-06 Type II method

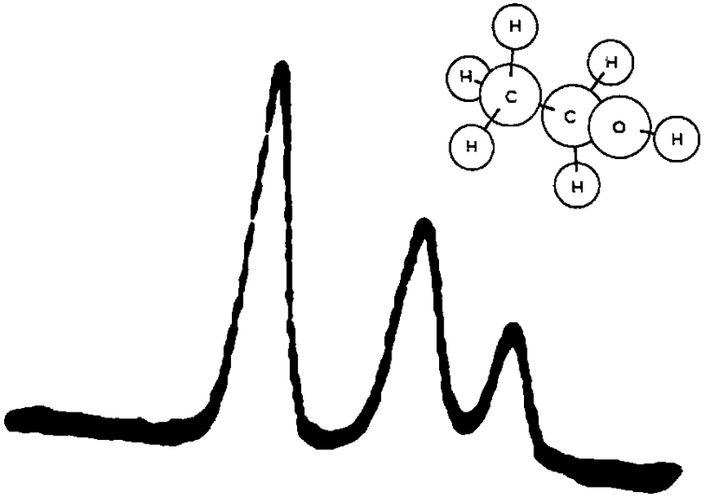
$^{18}O/^{16}O$ of wine water

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

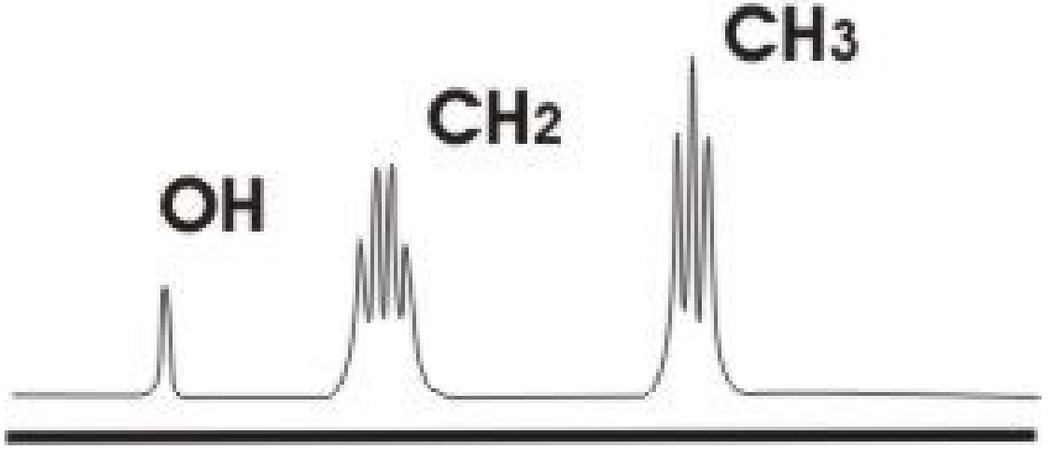
Method OIV-MA-AS2-12 Type II method

NMR

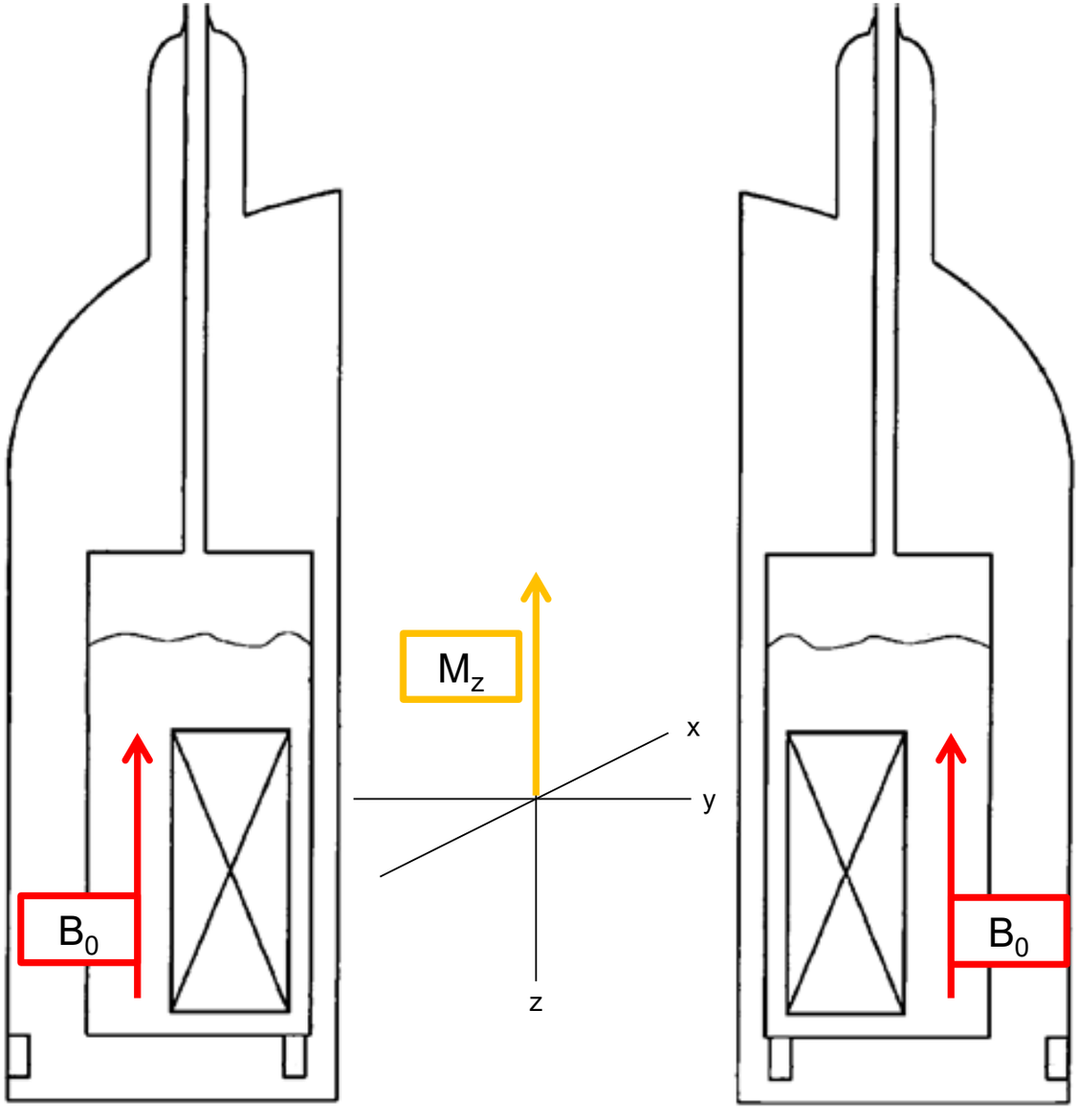
- Discovery of nuclear magnetic resonance by Edward Mills Purcell and Felix Bloch, Nobel price 1952



Early NMR-spectrum of ethanol (1951)
(source: www.wikipedia.org)



NMR



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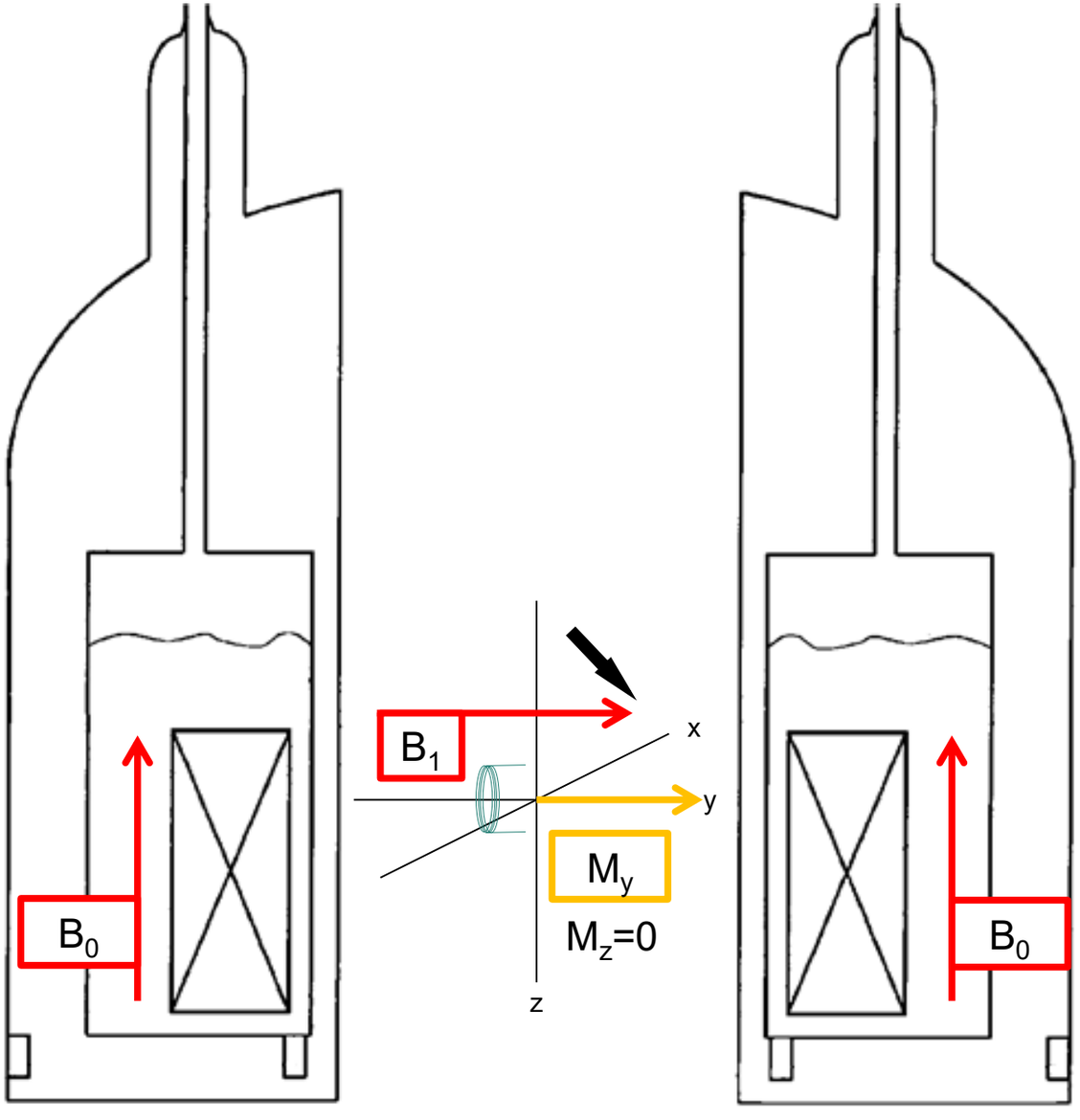

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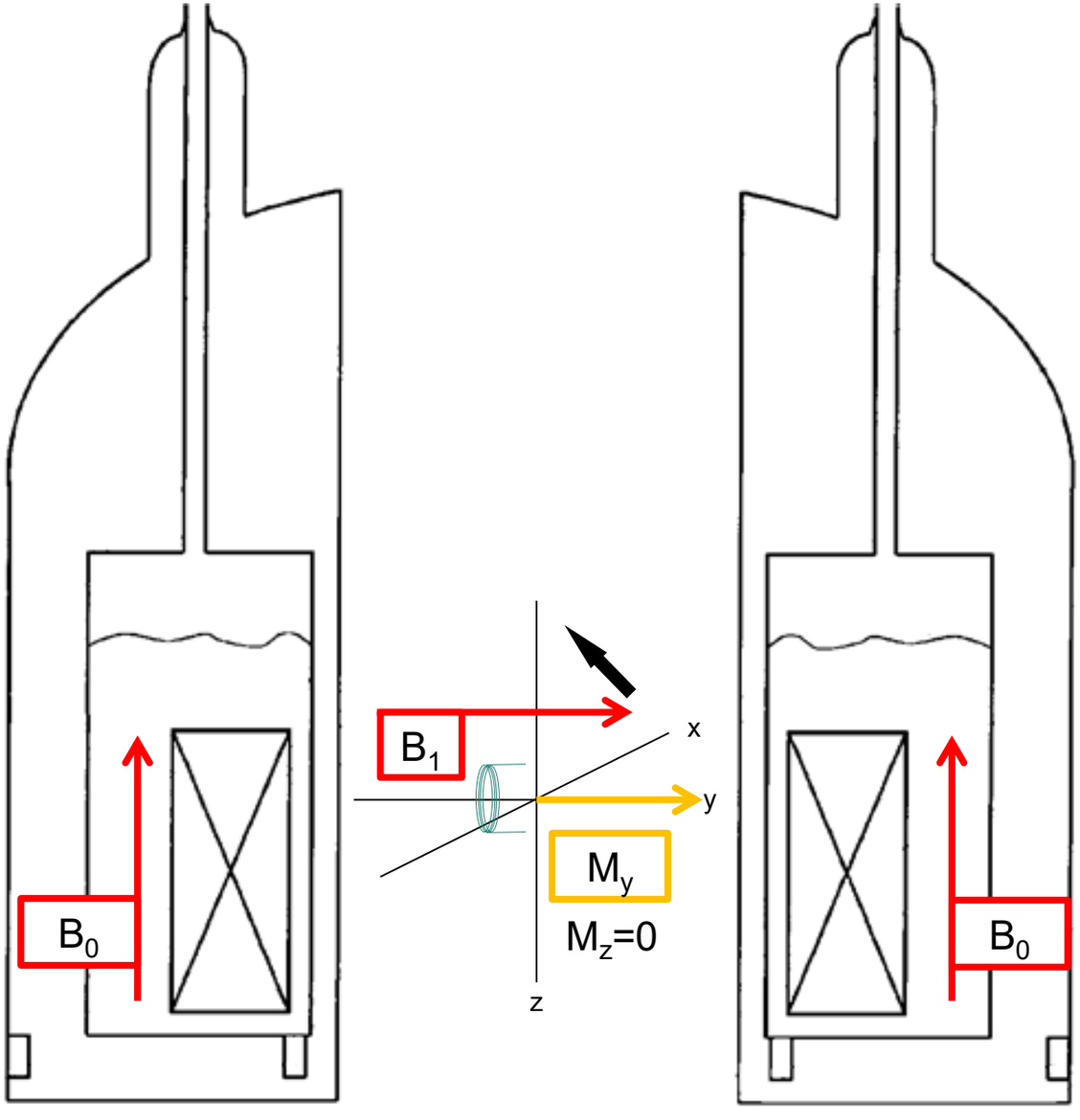

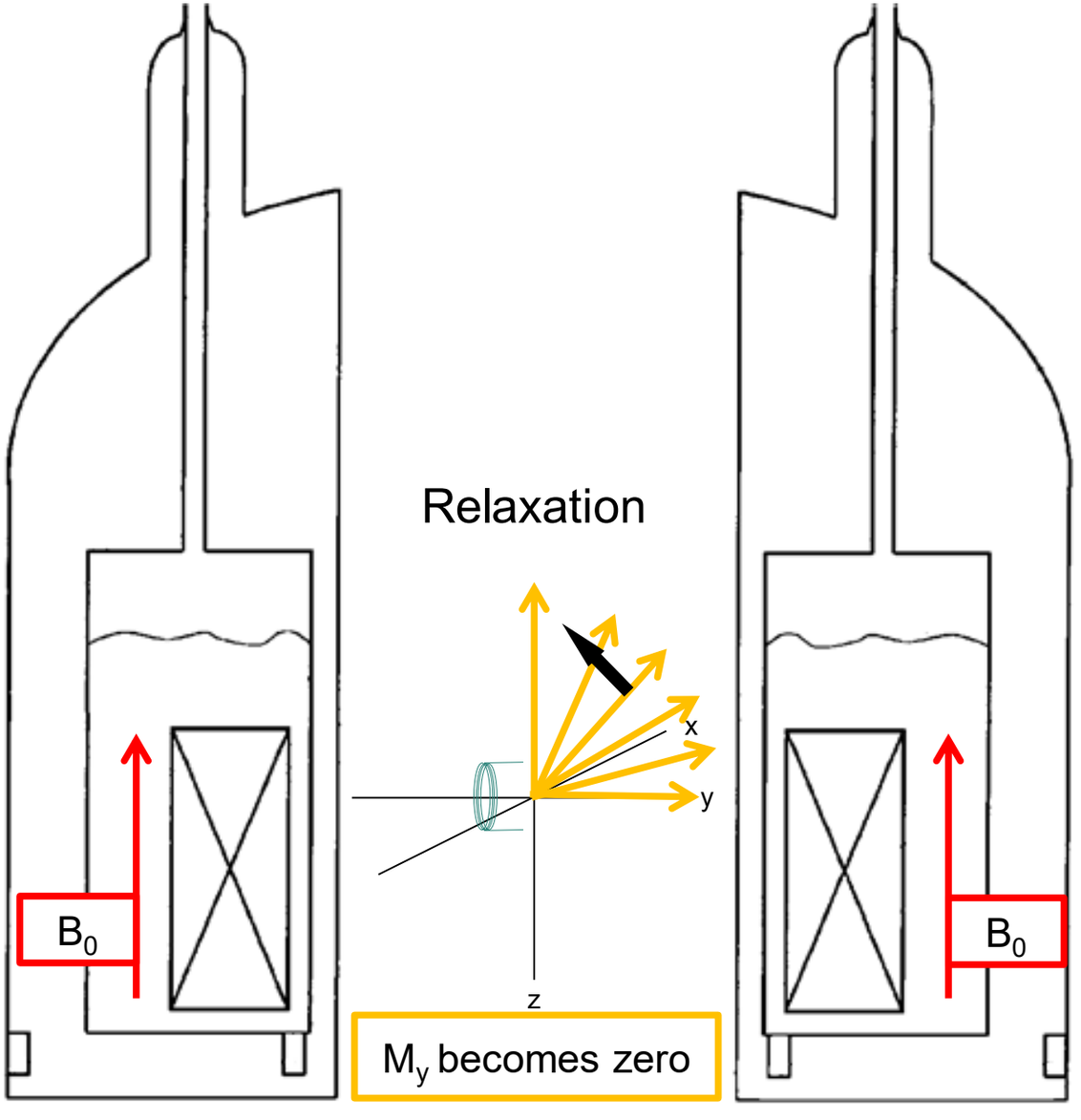

END Part A