

# TECHNICAL NOTE: 21-009

## Isotopologue Quantification

### Abstract

This technical note describes the quantification of the different isotopologues present in the deuterated reagents offered by Zeochem AG.

An isotopologue is a molecular entity that differs only in isotopic composition (number of isotopic substitutions). Quantitative  $^1\text{H}$ -NMR is used to measure the isotopic enrichment of the deuterated reagent. Deconvolution of the residual  $^1\text{H}$  signal is used to quantify different isotopologues in a sample.

All components present  $>0.1\text{w}\%$  are reported to 1 decimal place.

### Theoretical Background

Isotopologue is a type of isomer. Isotopologues share a chemical formula and bonding arrangement of atoms, but at least one atom has a different number of neutrons, i.e., the only difference between two isotopologues is the particular isotopes of the constituent elements that are present.

A deuterated reagent from Zeochem AG that contains more than one equivalent hydrogen atom will contain a distribution of different isotopologues, i.e. iodomethane- $\text{d}_3$  99.5%D does not contain 99.5% of fully deuterated iodomethane and 0.5% of iodomethane with no deuterium but a distribution of the different possible isotopologues.

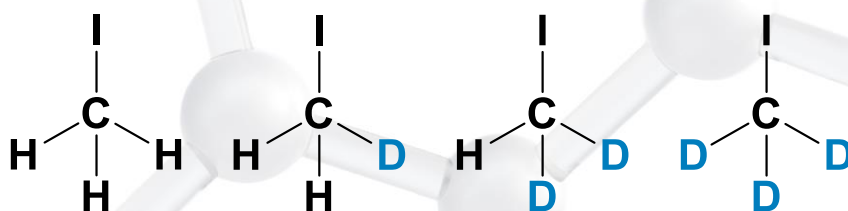


Figure 1. Four different isotopologues of iodomethane.

Isotopologues may be identified and quantified in  $^1\text{H}$ -NMR due to different splitting patterns caused by the coupling between  $^1\text{H}$  and  $^2\text{H}$  atoms.

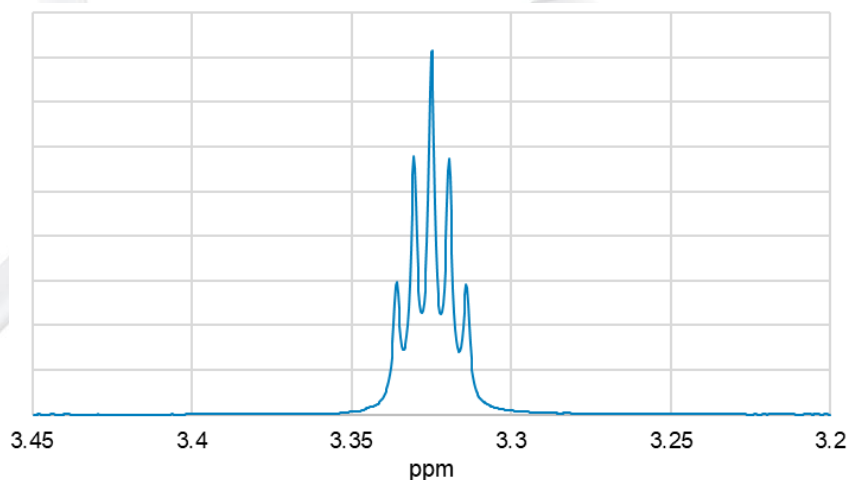


Figure 2. A coupling pattern observed for the residual  $^1\text{H}$  signal of methanol- $\text{d}_4$  in  $^1\text{H}$ -NMR.

## Trustable Measurements

### Fast results from internal measurements

All measurements are performed in-house by Zeochem AG at the manufacturing plant in Rütli, Switzerland.

### Traceable measurements

The quantitative NMR measurements are performed using Certified Reference Materials that conform to ISO 17034 and ISO/IEC 17025.