

# Tech Note

## Isotopologue Quantification

### Abstract

This tech 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 <sup>1</sup>H-NMR is used to measure the isotopic enrichment of the deuterated reagent. Deconvolution of the residual <sup>1</sup>H signal is used to quantify the different isotopologues in the sample.

Knowing the exact composition of materials can be important for certain applications. For instance, using our deuterated specialties to produce deuterium labelled APIs.

### Theoretical Background

Isotopologues are a type of isomer. They 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-d<sub>3</sub> 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.

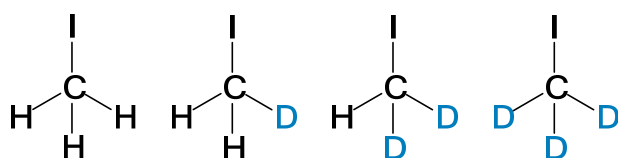
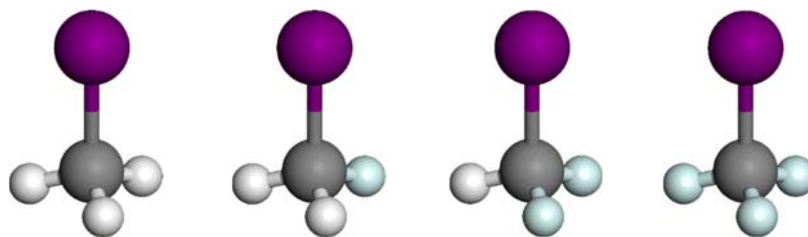


Fig. 1 Four different isotopologues of iodomethane



Different isotopologues may be identified in <sup>1</sup>H-NMR due to differing splitting patterns caused by the coupling between <sup>1</sup>H and <sup>2</sup>H. This allows for measurement and quantification of the different isotopologues.

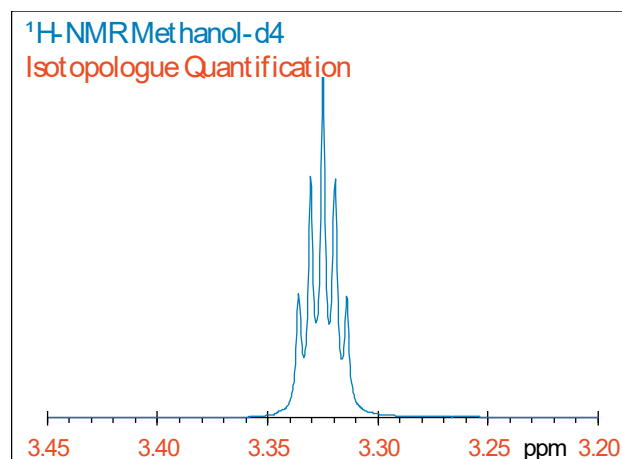


Fig. 2 Coupling pattern observed for the residual <sup>1</sup>H signal of methanol-d<sub>4</sub> in <sup>1</sup>H-NMR

### Trustable Measurements

#### Fast results from internal measurements

All measurements are an additional paid service 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.

#### Precise measurements

All present components with more than 0.1%W are reported to one decimal place.

### Different Products

We are happy to discuss the possibility of isotopologue quantification for all of our deuterated specialties with you.