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**NATIONAL STANDARD OF THE
PEOPLE'S REPUBLIC OF CHINA**

GB/T 45548-2025

**Determination of isotope abundance of deuterated reagents -
Nuclear magnetic resonance spectroscopy**

氘代试剂同位素丰度的测定 核磁共振波谱法

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Table of Contents

Foreword

1 Scope

2 Normative references

3 Terms and definitions

3.1 Stable isotope

3.2 Isotope abundance

3.3 Deuterated reagent

3.4 Deuterated sites

3.5 Deuterium-labeled compound

Foreword

This document is in accordance with the provisions of GB/T 1.1-2020 "Guidelines for standardization work Part 1: Structure and drafting rules for standardization documents" Drafting.

Please note that some of the contents of this document may involve patents. The publishing organization of this document does not assume the responsibility for identifying patents.

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Determination of isotopic abundance of deuterated reagents Nuclear magnetic resonance

spectroscopy

1 Scope

This document describes a method for determining the isotopic abundance of deuterated reagents using nuclear magnetic resonance spectroscopy.

This document applies to chloroform-D, dichloromethane-D₂, chlorobenzene-D₅, iodobenzene-D₅, bromobenzene-D₅, acetone-D₆, benzene-D₆, toluene-D₈, methanol-D₄, ethanol-D₆, heavy water, dimethyl sulfoxide-D₆, tetrahydrofuran-D₈, p-toluenesulfonyl methyl ester-D₃, bromobutanol-D₉, di(2-phthalic acid) butoxyethyl ester-D₄, methyl parahydroxybenzoate-branched-D₃, isovanillin-D₃, dimethyl phthalate-D₄, ethanol-D, acetic acid-D. Isotope abundance determination of 21 deuterated reagents (purity $\geq 98\%$). For the determination of isotope abundance of other deuterated reagents, please refer to this document.

2 Normative references

This document has no normative references.

3 Terms and definitions

The following terms and definitions apply to this document.

3.1 Stable isotope

An isotope of an element that does not undergo or is very unlikely to undergo radioactive decay, that is, an isotope of an element with a half-life greater than 10¹⁵ years.

[Source: GB/T 37750-2019, 3.1.12, modified]

3.2 Isotope abundance

The percentage of atoms of a particular isotope in a mixture of isotopes of an element to the total number of atoms of that element.

Note. It is expressed as atom% A, where A is the code for the element symbol of the specific isotope.

[Source: GB/T 37750-2019, 3.1.13, modified]

3.3 Deuterated reagent

A reagent that allows identification of a compound in which one or more hydrogen atoms have been replaced by a stable isotope, deuterium (²H or D).

[Source: GB/T 37750-2019, 3.3.11]

3.4 Deuterated sites

A site in a compound formed when hydrogen atoms with different chemical shifts are replaced by deuterium atoms.

Note. For example, benzene-D₆ has a single deuterium-labeled site; toluene-D₈ has multiple deuterium-labeled sites, including two deuterium-labeled sites, a deuterium-labeled methyl group and a deuterium-labeled phenyl group.

3.5 Deuterium-labeled compound

A compound labeled with deuterium atoms replacing all hydrogen atoms in the compound molecule.