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Deuterium Reagents

A Comprehensive Handbook for
Synthesis, Labeling, and Spectroscopy

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Introduction

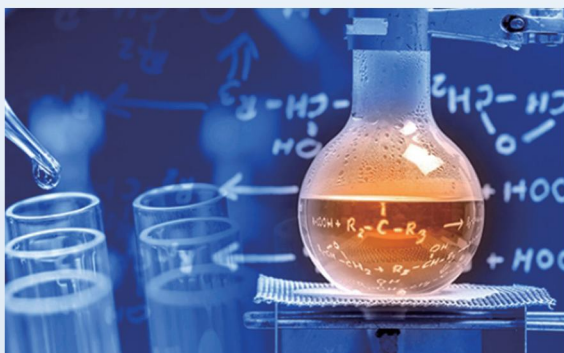
In the field of chemistry, isotopes play a crucial role in understanding the behavior and reactions of various elements. Among these isotopes, deuterium, a stable and non-radioactive isotope of hydrogen, has emerged as a powerful tool for researchers and practitioners alike. Its unique properties and versatility have paved the way for significant advancements in a wide range of scientific disciplines.

This handbook serves as a comprehensive guide to the world of deuterium reagents, providing an extensive collection of information, protocols, and applications. It aims to support chemists, researchers, and students in their exploration and utilization of deuterium reagents for various purposes, including synthesis, labeling, and spectroscopy.

We hope that this handbook will serve as an invaluable resource for chemists, researchers, and students seeking to explore the vast potential of deuterium reagents in their scientific endeavors. By providing a comprehensive overview of the specifications, we aim to facilitate the widespread adoption and effective utilization of deuterium reagents in diverse fields of chemistry.



Applications



Synthetic Chemistry

Deuterium reagents find extensive use in synthetic chemistry for the preparation of deuterated compounds. Deuterium labeling can provide valuable insights into reaction mechanisms, kinetics, and product distributions. It allows for the tracking of reaction pathways, identifying intermediates, and understanding the influence of isotopic effects on chemical transformations.



Medicinal Chemistry

Deuterium-labeled compounds have gained significance in drug discovery and development. Deuterium substitution at specific positions in drug molecules can enhance their metabolic stability, prolong their half-life, and improve their pharmacokinetic properties. Deuterium reagents enable the synthesis of deuterated drug candidates, leading to potential improvements in efficacy and reduced side effects.



Isotope Tracing

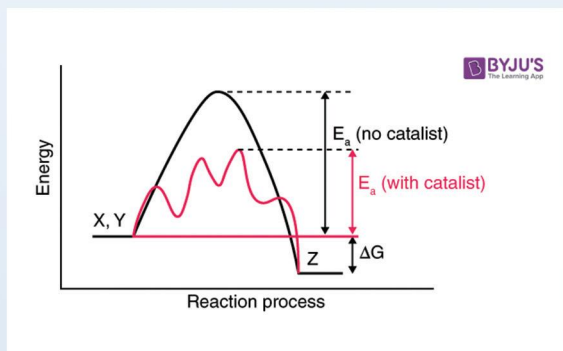
Deuterium reagents are used in isotope tracing experiments to study metabolic pathways and biochemical transformations. By replacing hydrogen atoms with deuterium in reactants or substrates, researchers can track the fate of deuterium-labeled atoms within biological systems. This technique aids in understanding metabolic fluxes, enzyme activities, and the dynamics of cellular processes.



Spectroscopy

Deuterium is widely employed in various spectroscopic techniques. In nuclear magnetic resonance (NMR) spectroscopy, deuterium-labeled compounds serve as valuable probes for elucidating molecular structures and dynamics. Deuterium exchange experiments provide insights into hydrogen bonding, solvent accessibility, and conformational changes in biomolecules. Additionally, deuterium is used in mass spectrometry and infrared spectroscopy for isotope ratio analysis and characterization of compounds.

Applications



Catalysis

Deuterium plays a crucial role in catalytic reactions, especially in hydrogenation and dehydrogenation processes. Deuterium-labeled substrates and reagents allow for the investigation of reaction mechanisms, surface interactions, and catalyst performance. Deuterium kinetic isotope effects provide valuable information about the rate-determining steps and transition states involved in catalytic reactions.



Environmental Studies

Deuterium reagents are utilized in environmental research to trace the sources and fate of water molecules. Isotope analysis of water samples, using deuterium as a marker, helps in studying hydrological cycles, groundwater dynamics, and understanding climate change patterns. Deuterium isotopic signatures are also employed in forensic investigations and tracing the origin of substances.

These applications highlight the versatility and significance of deuterium reagents in various scientific disciplines. The handbook will delve into each of these areas, providing detailed protocols, case studies, and practical guidance to facilitate their effective utilization.

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Chloroform-d

Cat. No	CAS	Size	Grade	Specification
C109595		0.6mL × 10	D, 99.8%	Proton NMR (Atom % D): 99.8-100% H₂O+D₂O (Karl Fischer): 0-0.01% Purity (GC): 99-100% Appearance: Colorless liquid Infrared spectrum: Conforms to Structure
		1g × 10		
		50g		
		100g		
		250g		
		100g × 10		
C109593		25g	(D, 99.8%) +1% V/V TMS	Proton NMR (Atom % D): 99.8-100% Water by Karl Fischer: 0-0.02% Mass Balance (V/V TMS): 0.95-1.2% Purity (GC): 99-100% Appearance: Colorless liquid Infrared spectrum: Conforms to Structure
		50g		
		100g		
		500g		
C109594	865-49-6	1g × 10	(D, 99.8%) +0.03% V/V TMS	Proton NMR (Atom % D): 99.8-100% Water by Karl Fischer: 0-0.03% Mass Balance (V/V TMS): 0.026-0.04% Purity (GC): 99-100% Appearance: Colorless liquid Infrared spectrum: Conforms to Structure
		50g		
		100g		
		500g		
C122876		10g	100%, 99.96 atom % D	Proton NMR (Atom % D): 99.96-100% Water by Karl Fischer: 0-0.01% Purity (GC): 99-100% Appearance: Colorless liquid Infrared spectrum: Conforms to Structure
		0.75mL × 10		
		1mL × 10		
		50g		

Toluene-d8

Cat. No	CAS	Size	Grade	Specification
T102274		1g	D, 99.60%	Proton NMR (Atom % D): 99.6-100% Water by Karl Fischer: 0-0.01% Purity (GC): 99-100% Appearance: Colorless liquid
		5g		
		0.75mL × 10		
		1mL × 10		
		10g		
		25g		
T102275	2037-26-5	0.5mL	D, 99.94%	Proton NMR (Atom % D): 99.94-100% Water by Karl Fischer: 0-0.01% Purity (GC): 99-100% Appearance: Colorless liquid
		1mL		
		0.5mL × 5		
		0.75mL × 5		
		5mL		
		0.5mL × 10		
T102276		0.75mL × 10	D, 99.5% (0.03% TMS)	Proton NMR (Atom % D): 99.5-100% Water by Karl Fischer: 0-0.01% Purity (GC): 99-100% Appearance: Colorless liquid
		10g		

Methanol-d4

Cat. No	CAS	Size	Grade	Specification
M102264		0.6mL × 2	D, 99.8% (0.05% v/v TMS)	Proton NMR (Atom % D): 99.8-100% Water by Karl Fischer: 0-0.025% Mass Balance (V/V TMS): 0.046-0.06% Purity (GC): 99-100% Appearance: Colorless liquid
		0.6mL × 10		
		5g		
		10g		
		25g		
		50g		
M102262	811-98-3	0.5mL × 2	D, 99.8%	Proton NMR (Atom % D): 99.8-100% Water by Karl Fischer: 0-0.025% Purity (GC): 99-100% Appearance: Colorless liquid
		0.75mL × 2		
		0.5mL × 10		
		0.75mL × 10		
		1g × 10		
		5g		
		25g		
		100g		
		M140114		
0.75mL × 10				
1mL × 10				
1g				
5g				
25g				

Ethanol-d

Cat. No	CAS	Size	Grade	Specification
E102260	1516-08-1	1g	D, 99%, anhydrous grade	Proton NMR (Atom % D): 99-100% H₂O+D₂O (Karl Fischer): 0-1% Appearance: Colorless liquid
		5g		
		1g × 5		
E304986	925-93-9	5g	d1, (D, 99%) (<6% D ₂ O)	Isotopic purity (Atom % D): 99.5-100% Water by Karl Fischer (D₂O): 0-5% NMR Spectrum ¹H: Conforms to Structure Appearance: Colorless liquid
		25g		
		50g		
		100g		

Deuterium Chloride

Cat. No	CAS	Size	Grade	Specification
D304594	7698-05-7	10g	35 wt. % in D ₂ O, ≥99 atom % D	Isotopic Purity: 99-100% Appearance: Colorless liquid Concentration (Titration by NaOH): 34-37%
		50g		

Acetonitrile-d3

Cat. No	CAS	Size	Grade	Specification
A100969		0.75mL × 5	(D, 99.96%)	Proton NMR (Atom % D): 99.96-100% Water by Karl Fischer: 0-0.02% Purity (GC): 99-100% Appearance: Colorless liquid
		0.5mL × 10		
		0.6mL × 10		
		0.75mL × 10		
		5mL		
		25mL		
A100970	2206-26-0	0.6mL × 10	(D, 99.8%) (0.03% v/v TMS)	Proton NMR (Atom % D): 99.8-100% Water by Karl Fischer: 0-0.02% Mass Balance (V/V TMS): 0.026-0.04% Purity (GC): 99-100% Appearance: Colorless liquid
		5g		
		10g		
		25g		
A100968		0.5mL × 10	(D, 99.8%)	Proton NMR (Atom % D): 99.8-100% Water by Karl Fischer: 0-0.02% Purity (GC): 99-100% Appearance: Colorless liquid
		0.6mL × 10		
		0.75mL × 10		
		1g × 10		
		5g		
		10g		
		25g		
50g				

Pyridine-d5

Cat. No	CAS	Size	Grade	Specification
P140017		0.5mL × 10	(D, 99.5%) +0.03% V/V TMS	Proton NMR (Atom % D): 99.5-100% Water by Karl Fischer: 0-0.05% TMS, 0.03% v/v: conform Appearance: Colorless liquid
		5g		
		10g		
P113720	7291-22-7	0.6mL × 10	(D, 99.5%) +0.05% V/V TMS	Proton NMR (Atom % D): 99.5-100% Water by Karl Fischer: 0-0.05% Mass Balance (V/V TMS): 0.04-0.06% Appearance: Colorless liquid
		1g × 10		
		5g		
		10g		
		25g		
P113721		0.5mL × 10	(D, 99.5%)	Proton NMR (Atom % D): 99.5-100% Water by Karl Fischer: 0-0.05% Appearance: Colorless liquid
		1mL × 10		
		1g		
		5g		
		10g		
25g				

N,N-Dimethylformamide-d7

Cat. No	CAS	Size	Grade	Specification
N102258	4472-41-7	0.6mL	D, 99.5%	Proton NMR (Atom % D): 99.5-100% Water by Karl Fischer: 0-0.05% Purity (GC): 99-100% Appearance: Colorless liquid
		1g		
		5g		
		1g×5		
		10mL		

Benzene-d6

Cat. No	CAS	Size	Grade	Specification
B100912	1076-43-3	0.5mL×10	D, 99.5%	Proton NMR (Atom % D): 99.5-100% Water by Karl Fischer: 0-0.03% Purity (GC): 99-100% Appearance: Colorless liquid Infrared spectrum: Conforms to Structure
		0.75mL×10		
		5g		
		10g		
		25g		
		50g		
		100g		
		1g×10		
B100913	1076-43-3	0.6mL×10	D, 99.6% (0.03% v/v TMS)	Water by Karl Fischer: 0-0.03% Mass Balance (V/V TMS): 0.026-0.04% Purity (GC): 99-100% Appearance: Colorless liquid Proton NMR spectrum: Conforms to Structure
		10g		
		25g		
		50g		
B100918	1076-43-3	0.5mL×5	D, 99.96%	Proton NMR (Atom % D): 99.96-100% Water by Karl Fischer: 0-0.01% Purity (GC): 99-100% Appearance: Colorless liquid
		0.75mL×5		
		0.5mL×10		
		0.75mL×10		
		1mL×10		
		5mL		
		25mL		
B100914	1076-43-3	0.75mL×2	D, 99.96% (0.03% v/v TMS)	Water by Karl Fischer: 0-0.01% Mass Balance (V/V TMS): 0.026-0.04% Purity (GC): 99-100% Appearance: Colorless liquid Proton NMR spectrum: Conforms to Structure
		0.75mL×10		

Acetone-d6

Cat. No	CAS	Size	Grade	Specification
A100962	666-52-4	1mL × 10	(D, 99.9%) + 0.03 % (v/v) TMS	Proton NMR (Atom % D): 99.85-100% Water by Karl Fischer: 0-0.05% Mass Balance (V/V TMS): 0.026-0.4% Purity (GC): 99-100% Appearance: Colorless liquid
		10mL		
		50mL		
A100963		0.6mL × 10	(D, 99.96%) (+0.03% V/V TMS)	Proton NMR (Atom % D): 99.96-100% Water by Karl Fischer: 0-0.05% Mass Balance (V/V TMS): 0.026-0.4% Purity (GC): 99-100% Appearance: Colorless liquid
		0.75mL × 10		
		5mL		
		25mL		
A100965		0.6mL × 10	(D, 99.9%)	Proton NMR (Atom % D): 99.9-100% Water by Karl Fischer: 0-0.05% Purity (GC): 99-100% Appearance: Colorless liquid
		10mL		
		25mL		
		100mL		
A123143		0.5mL × 10	(D, 99.96%)	Proton NMR (Atom % D): 99.96-100% Water by Karl Fischer: 0-0.05% Purity (GC): 99-100% Appearance: Colorless liquid
	0.75mL × 10			
	1mL			
	1mL			
	25mL			

Trifluoroacetic Acid-d

Cat. No	CAS	Size	Grade	Specification
T109783	599-00-8	0.5mL × 10	D, 99.5%	Proton NMR (Atom % D): 99.5-100% Water by Karl Fischer: 0-0.5% Appearance: Colorless liquid
		0.75mL × 10		
		1g × 10		
		5g		
		10g		
		25g		
T109782		5g	99.5 atom % D +0.03%TMS, for use in NMR	Proton NMR (Atom % D): 99.5-100% Water by Karl Fischer: 0-0.5% Appearance: Colorless liquid
		10g		
		25g		

Sulfuric Acid-d

Cat. No	CAS	Size	Grade	Specification
S102269	13813-19-9	5g	(D, 99.5%) 96% IN D2O	Proton NMR (Atom % D): 99.5-100% Purity (Titration by NaOH): 95.5-104.5% Appearance: Colorless liquid NMR (¹ H-NMR): complies
		10g		
		25g		
		50g		

Dimethyl Sulfoxide-d6

Cat. No	CAS	Size	Grade	Specification
D106263		5g	D. 99.9%	Proton NMR (Atom % D): 99.9-100% Water by Karl Fischer: 0-0.03% Purity (GC): 99-100% Appearance: Colorless liquid Infrared spectrum: Conforms to Structure
		10g		
		25g		
		50g		
		0.6mL × 10		
		0.75mL × 10		
D106264		5g	D.99.9% +0.03%TMS	Proton NMR (Atom % D): 99.9-100% Water by Karl Fischer: 0-0.03% Mass Balance (V/V TMS): 0.026-0.04% Purity (GC): 99-100% Appearance: Colorless liquid Infrared spectrum: Conforms to Structure Proton NMR Spectrum: Conforms to Structure
		10g		
		25g		
		50g		
D106265	2206-27-1	5g	D. 99.9% +0.05%TMS	Proton NMR (Atom % D): 99.9-100% Water by Karl Fischer: 0-0.03% Mass Balance (V/V TMS): 0.046-0.06% Purity (GC): 99-100% Appearance: Colorless liquid Infrared spectrum: Conforms to Structure
		10g		
		25g		
		50g		
		1g × 10		
D106266		0.6mL × 10	D. 99.9% +1%TMS	Proton NMR (Atom % D): 99.9-100% Water by Karl Fischer: 0-0.03% Mass Balance (V/V TMS): 0.95-1.2% Purity (GC): 99-100% Appearance: Colorless liquid Infrared spectrum: Conforms to Structure
		0.75mL × 10		
		1g × 10		
		5g		
		10g		
		25g		
50g				

Deuterium Oxide

Cat. No	CAS	Size	Grade	Specification
D113906		25g	99 atom % D	Proton NMR (Atom % D): 99-100% Appearance: Colorless liquid NMR (¹ H-NMR): complies
		100g		
		1kg		
D113904	7789-20-0	0.55mL × 10	99.9 atom % D	Proton NMR (Atom % D): 99-100% Appearance: Colorless liquid
		25g		
		100g		
		250g		
		500g		
1kg				

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