



For the Broadest
Range of NMR
Solvents and Tubes

Add  Aldrich

Aldrich® Chemistry – Your Source for NMR Solvents, Tubes and Accessories

Only Aldrich Chemistry offers the greatest breadth of NMR products available from world class manufacturers such as:



Our NMR products are conveniently grouped into four broad categories to quickly help determine the best solvents and tubes to meet your requirements.

High Resolution NMR

- High field experiments
- Temperature gradients
- Multi-dimensional analysis
- Biological compounds with high molecular weight

Routine NMR

- 1D NMR experiments
- Small organic molecules (molecular weight typically <1500)
- Ambient temperature testing
- Qualitative vs. quantitative results

High Throughput NMR

- Sequential data acquisition for a series of samples
- Useful in drug discovery process
- Typically disposable tubes

Air-Sensitive NMR

- Air- and moisture-sensitive samples
- Perform under vacuum and inert gas
- Controlled environments



High Resolution NMR

High Resolution NMR requires only the highest quality NMR solvents and tubes for critical shimming quality.

Aldrich® 100% NMR Solvents

In high resolution NMR, it is critical to choose a solvent with high chemical and isotopic purity. Aldrich "100%" NMR solvents are the highest isotopically enriched solvents sold and will not interfere with your desired level of detection.

"100%", 99.96 atom % D solvents

Product No.	Solvent
175862	Acetone-d ₆
233323	Acetonitrile-d ₃
175870	Benzene-d ₆
151858	Chloroform-d
151890	Deuterium oxide
233366	Dichloromethane-d ₂
156914	Dimethyl sulfoxide-d ₆
194166	Methanol-d ₄
177970	Pyridine-d ₅
233382	Toluene-d ₈

*100% D solvents are offered in multiple sizes and packaging configurations.

"Extra" enriched D₂O solvents

Product No.	Solvent
613398	D ₂ O, Extra, 99.994 atom % D
191701	D ₂ O, 99.990 atom % D

Premium NMR Tubes

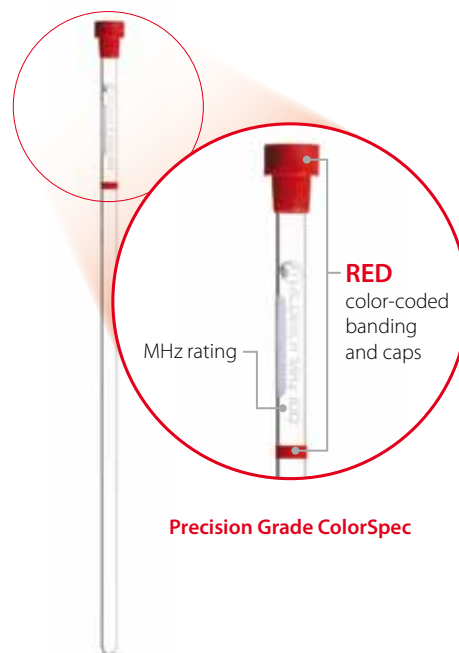
These tubes have the tightest specifications for concentricity and camber, ensuring a well-balanced spin rate and the highest shimming quality.

ASTM type 1, Class A thin wall (0.38 mm) borosilicate glass

- Aldrich Precision Grade ColorSpec® NMR tubes
RED color-coded banding and caps, and a MHz rating that allows for instant visual identification.
- Norell® Select Series™ NMR tubes
- Shigemi NMR Microtubes
Magnetic susceptibility matched to CDCl₃, CD₃OD, DMSO-d₆, or D₂O for best resolution.
- Wilmad® Precision Grade NMR tubes

For a complete listing of all available High Resolution NMR solvents and tubes, visit

Aldrich.com/highresnmr



Routine NMR

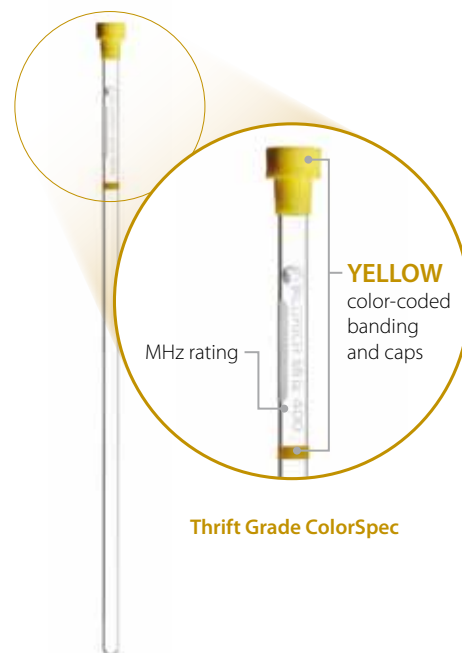
Routine NMR is performed at ambient temperatures where shimming quality is less critical. Due to the nature of these experiments, routine NMR is more commonly performed to collect qualitative, rather than quantitative, data.

Aldrich® High Purity NMR Solvents

Standard purity solvents are suitable for routine NMR. Additionally, Aldrich Chemistry supplies solvents with TMS or other stabilizers. Packaging configurations include ampule packs, glass bottles, serum bottles and Aldrich Sure/Seal™ bottles.

Prod. No.	Solvent	atom % D
151785	Acetic acid-d ₄	99.5
151793	Acetone-d ₆	99.9
151807	Acetonitrile-d ₃	99.8
151815	Benzene-d ₆	99.6
151823	Chloroform-d	99.8
151866	Cyclohexane-d ₁₂	99.6
151882	Deuterium oxide	99.9
444324	Dichloromethane-d ₂	99.9
189979	<i>N,N</i> -Dimethyl formamide-d ₇	99.5

Prod. No.	Solvent	atom % D
151874	Dimethyl sulfoxide-d ₆	99.9
186406	1,4-Dioxane-d ₈	99
186414	Ethanol-d ₆	99.5
151947	Methanol-d ₄	99.8
532975	Pyridine-d ₅	99.5
184314	Tetrahydrofuran-d ₈	99.5
434388	Toluene-d ₈	99.6
152005	Trifluoroacetic acid-d	99.5



Thrift Grade ColorSpec

Economy NMR Tubes

NMR tubes for routine applications allow for slightly greater variance of concentricity and camber than precision tubes and have a greater impact on shimming quality. With proper handling and sample preparation, they provide sufficient quality for most standard analysis.

ASTM Type 1, Class B medium wall (0.43 mm) borosilicate glass

- Aldrich Thrift Grade ColorSpec® NMR tubes
YELLOW color-coded banding and caps, and a MHz rating that allows for instant visual identification.
- Norell® Standard Series™ NMR tubes
- Wilmad® Economy Grade NMR tubes

For a complete listing of all available Routine NMR solvents and tubes, visit

Aldrich.com/routinenmr

High Throughput NMR

High Throughput NMR is commonly described by use of automatic sample changers to acquire data sequentially from a series of samples. Due to the large volume of samples, these NMR tubes are typically disposable.

Aldrich® Solvents for High Throughput NMR

Depending on the experiment and desired signal to noise ratio, either Aldrich Chemistry's "100%" deuterated solvents or standard NMR solvents may be appropriate. References to these solvent listings can be found in the previous high resolution and routine NMR sections.

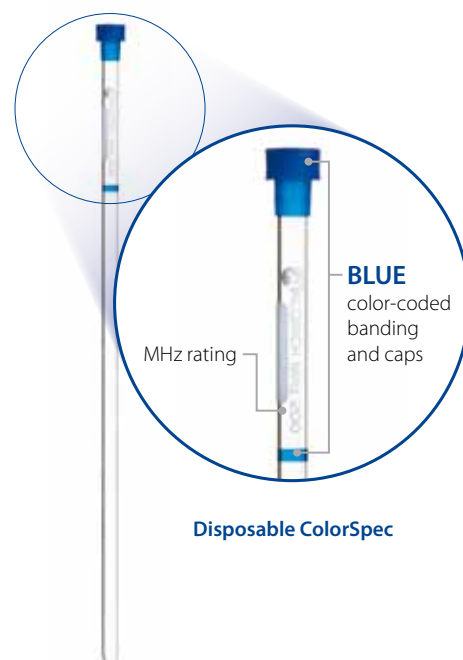
In choosing the correct solvent purity, it is also important to know the amount of sample available and the desired concentration. A useful chart in determining the isotopic purity required can be found in the technical reference section of this brochure.

High Throughput NMR Tubes

Type 1, Class A or Class B borosilicate glass. Sold in larger packs (50 or 100) and are disposable.

- Aldrich Disposable ColorSpec® NMR tubes
BLUE color-coded banding and caps, and a MHz rating that allows for instant visual identification.
- Norell® Standard Series™ NMR tubes
- Wilmad® Economy Grade NMR tubes
- Bruker Match™ tubes
- Norell® Sample Vault Series™ NMR tubes
For Bruker® SampleJet™ robotic high-throughput automated systems.

For a complete listing of all available High Throughput NMR solvents and tubes, visit Aldrich.com/htpnmr



Disposable ColorSpec

Air-Sensitive NMR

Some NMR experiments require the utmost carefully controlled environments, often under vacuum and inert gas. The NMR products below highlight how Aldrich® Chemistry can help you perform critical air- and moisture-sensitive NMR analysis.

Anhydrous NMR Solvents

Water contamination is one of the most common problems of NMR spectroscopy. Aldrich Chemistry anhydrous solvents minimize or eliminate any interference from water peaks.

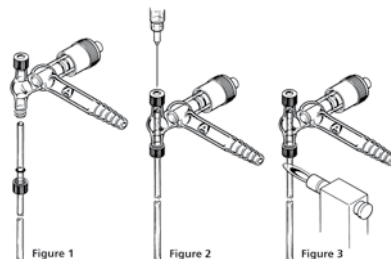
Prod. No.	Solvent
570680	Benzene-d ₆ , 99.6 atom % D (water <10 ppm)
570699	Chloroform-d, 99.8 atom % D (water <10 ppm)
569585	DMSO-d ₆ , 99.9 atom % D (water <50 ppm)
570729	Methanol-d ₄ , 99.8 atom % D (water <50 ppm)
570710	Toluene-d ₈ , 99.6 atom % D (water <10 ppm)

Specialty NMR Tubes and Accessories

Offering a full range of products designed to eliminate the effects of exposure to air and moisture.

- **Wilmad® screw-cap NMR tubes (Z271950)**
Open-top, screw-thread cap with a PTFE/silicone septum that permits addition of reactants or samples via syringe.
- **Wilmad quick pressure valve NMR tubes (Z562866)**
Designed to simplify the process when performing studies in catalysis, gas-liquid phase reactions, air-sensitive samples and elevated temperature experiments.
- **Wilmad low pressure/vacuum valved NMR tubes (Z568139)**
A convenient flame-free sealing solution for air-sensitive or volatile liquid samples.
- **Aldrich 5 mm NMR tube filling manifold (Figures 1-3)**
Convenient, easy system for flame sealing air- and moisture-sensitive NMR tubes. Manifolds available in 1 port, 2 port and 5 port configurations.
- **Aldrich NMR-tube Dewar flask**
Designed for freezing NMR samples in vacuum-thaw work.
- **eVol® electronic syringe NMR starter kit**
The eVol NMR Edition kit allows accurate manipulation of small volumes of NMR samples enabling dilution directly in the analysis tube – even in tubes with the smallest internal diameters.

- **Precision Seal® rubber septa caps for 5 mm tubes**
Provides a penetration point for cannulation and a dual seal inside the tube.



Precision Seal
rubber septa
caps for 5 mm
tubes

For a complete listing of all available Air-Sensitive NMR solvents, tubes and NMR accessories, visit Aldrich.com/airsensnmr

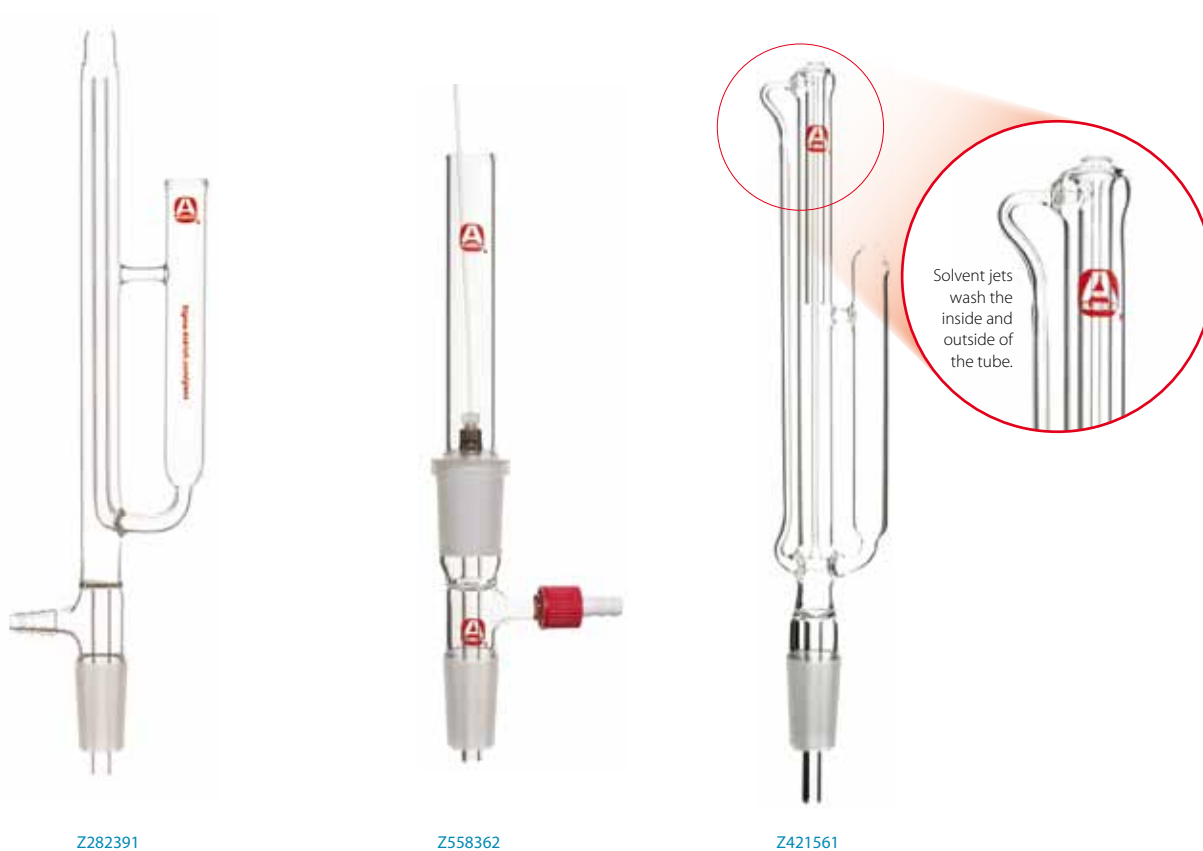


eVol electronic syringe NMR starter kit
Kit contains items shown in image.

Innovative NMR Tube Cleaners

Aldrich® Chemistry supports NMR scientists with a broad offering of NMR tube cleaners.

- **Aldrich single stage NMR tube cleaner (Z282391)**
With various joint sizes – 24/40, 29/32 and tooled end.
- **Aldrich SafetyBarb® NMR tube cleaner (Z558362)**
Inner PTFE wash tube with Luer connection prevents NMR tube breakage during the cleaning process. Detaches for thorough cleaning or replacement. SafetyBarb vacuum connection.
- **Aldrich dual-action NMR tube cleaner (Z421561)**
Washes tubes inside and out simultaneously. Available in single and multi-position configurations.



For a complete listing of all Aldrich NMR tube cleaners, visit

[Aldrich.com/nmrcleaners](https://www.aldrich.com/nmrcleaners)

NMR Spectral References

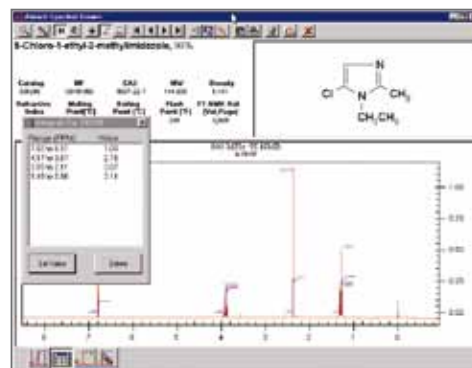
Aldrich® Chemistry also assists NMR chemists with the technical data required for their research.

Aldrich Spectral Viewer™

This electronic reference book on CD-ROM contains thousands of spectra from the Aldrich spectral libraries. This easy-to-use software program is more powerful than a printed book, allowing text and data field searching and the manipulation, printing, and exporting of spectra.

Currently, we offer two ¹³C and ¹H FT-NMR libraries. The standard library contains 11,800 compounds; the supplemental library contains 3,500 compounds. Academic versions are available.

In addition, we offer FT-IR, ATR-IR and Raman libraries. The libraries can be used individually or can be combined to create a powerful, electronic reference. A single user interface handles all libraries, simplifying the use of the software. In addition, the Spectral Viewer is expandable so when new spectral libraries are released, they can be easily added to the software.



To find out more about the Aldrich Spectral Viewer, visit Aldrich.com/spectralviewer

ACD/Spectrus Processor and the Sigma-Aldrich® Library

Access all your analytical data and the Aldrich FT-NMR Library in one integrated software package.

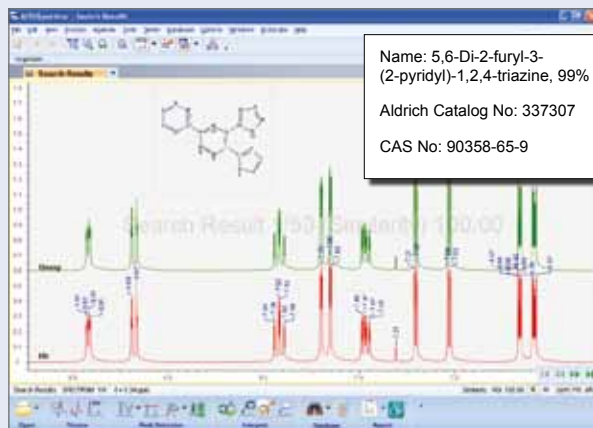
- Process
- Analyze
- Search
- Verify



ACD/Spectrus Processor is an all-in-one processing, interpretation, and reporting software for NMR, LC/MS, IR, and other analytical techniques.

For more information on ACD/Spectrus Processor, visit acdlabs.com/aldrich

Visionary Software  Advancing Research



Reference Standards

In addition to our high quality solvent product line, we offer a wide range of NMR reference standards needed to verify instrument performance.

NMR Reference Standards

Sigma-Aldrich® NMR reference standards allow users to monitor key operational parameters such as PW90, sensitivity, resolution and line shape.

Product No.	Solution	Application	Tube size (O.D. x L)
487163	1% Chloroform solution in acetone-d ₆ (99.9 atom % D)	¹ H line shape	5 mm x 8 in.
487104	0.1% Ethylbenzene solution, 0.01% TMS in chloroform-d (99.8 atom % D)	¹ H sensitivity	5 mm x 8 in.
611905	40% 1,4-Dioxane solution, 5 mg/mL chromium(III) acetylacetonate in benzene-d ₆ (99.6 atom % D)	¹³ C PW90, sensitivity	5 mm x 8 in.

These are three of the most common NMR reference standards. In addition, Aldrich Chemistry offers standards for nitrogen, fluorine and phosphorus sensitivity. Standards are also available in a multitude of lengths and outer diameters. Aldrich Chemistry is also able to produce many custom standards. Contact your local Aldrich Chemistry representative for more information.

For a complete listing of available NMR reference standards, visit

Aldrich.com/nmrrefstd

TraceCERT® Certified Reference Materials (CRMs) for quantitative NMR (qNMR)

Fluka® provides a set of NIST traceable CRMs produced under ISO/IEC 17025 and ISO Guide 34, intended for use as internal standards for quantitative NMR. The products cover a wide range of ppm values and solvents as shown in the table below. The general package size is 5 g.

Product No.	Substance	Chemical Shifts	Solubility			
			D ₂ O	MeOD	CDCl ₃	DMSO-d ₆
15639	3,5-Dinitrobenzoic acid	9.2 ppm				●
06185	Benzoic acid	7.4 - 8.2 ppm		●		●
41867	Dimethyl sulfone	3.2 ppm	●		●	●
14659	Potassium phthalate monobasic	~ 7 - 8 ppm	●	●		
03826	Calcium formate	~ 7.5 - 8.5 ppm	●			
92816	Maleic acid	6.2 ppm	●	●		●
40384	1,2,4,5-Tetrachloro-3-nitrobenzene	7.8 - 8.4 ppm			●	●
06856	Duroquinone	2 ppm			●	
74658	1,2,4,5-Tetramethylbenzene	2.3 + 7.0 ppm			●	
07038	Dimethyl terephthalate	3.9 + 8.1 ppm		●	●	●

To find out more about organic TraceCERT products, visit

Aldrich.com/organiccrm

NMR Technical References

Choosing the Correct Isotopic Purity

Selecting the right NMR solvent and isotopic purity is largely dependent on the amount of sample you have. When choosing the isotopic purity of your deuterated solvent for proton NMR, it is important to avoid any interfering resonances. The table below serves as a rough guide for selecting isotopic purity of NMR solvents for your sample.

Sample Mass MW=250	Molar Sample Concentration	Min. Solvent Isotopic Purity
12.5 mg	0.1 M	99.0%
6 mg	0.05 M	99.5%
2.5 mg	0.02 M	99.8%
1 mg	0.005 M	99.95%

*Reprinted with permission of Wilmad-LabGlass.

"Double Water Peaks" in Deuterated NMR Solvents

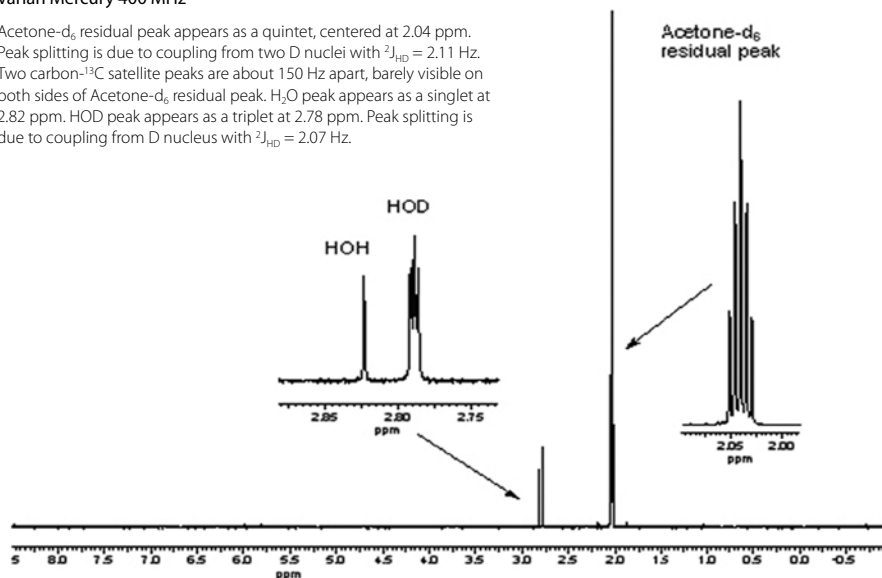
In deuterated NMR solvents, such as CDCl_3 , Acetone- d_6 , CD_3CN , and $\text{DMSO}-d_6$, trace water is inevitable due to the manufacturing process and solvent storage conditions. Generally speaking, water takes three forms in a deuterated solvent environment: HOH, HOD, and DOD. In the proton NMR spectrum of a pure NMR solvent, both the HOH and HOD peaks are observed, but not the DOD.

In a proton NMR Spectrum, HOH appears as a singlet. However, due to coupling from the D nucleus which has a nuclear spin quantum number $I = 1$, HOD appears as a triplet. The observed splitting ${}^2J_{\text{HD}}$ of the HOD peak is about 1-2 Hz. The chemical environments of the protons in HOH and HOD are similar, but not identical. Therefore, the HOH and HOD peaks appear to be close in chemical shift, but not overlapped. They are typically 0.03 ppm apart.

Below is a NMR spectrum showing the HOH and HOD peaks for Acetone- d_6 . The reported chemical shifts and couplings constants are directly measured from the spectrum.

Proton NMR Spectrum of Acetone- d_6 Solvent NMR Instrument: Varian Mercury 400 MHz

Acetone- d_6 residual peak appears as a quintet, centered at 2.04 ppm. Peak splitting is due to coupling from two D nuclei with ${}^2J_{\text{HD}} = 2.11$ Hz. Two carbon- ${}^{13}\text{C}$ satellite peaks are about 150 Hz apart, barely visible on both sides of Acetone- d_6 residual peak. H_2O peak appears as a singlet at 2.82 ppm. HOD peak appears as a triplet at 2.78 ppm. Peak splitting is due to coupling from D nucleus with ${}^2J_{\text{HD}} = 2.07$ Hz.



Use and Handling of NMR Solvents

Most deuterated NMR solvents readily absorb moisture. To minimize the chance of water contamination, use carefully dried NMR tubes and handle NMR solvents in a dry atmosphere.

How to Obtain a Nearly Moisture-free Surface

1. Dry glassware at ~ 150 °C for 24 hours and cool under an inert atmosphere.
2. Rinse the NMR tube with the deuterated solvent prior to preparing the sample. This allows for a complete exchange of protons from any residual moisture on the glass surface.
3. For less demanding applications, a nitrogen blanket over the sample preparation setup may be adequate.

How to Avoid Sources of Impurities and Chemical Residues

1. Use clean, dry glassware and PTFE accessories.
2. Use a vortex mixer instead of shaking the tube contents. The latter action can introduce contaminants from the NMR tube cap.
3. Residual chemical vapor from equipment can be a source of impurities; residual acetone in pipette bulbs is a common example.

How to Remove Solvent Residue

1. Protonated solvent residue can be removed by co-evaporation.
2. Use a small quantity of the desired deuterated solvent, a brief high-vacuum drying (5-10 min), and then prepare the NMR sample.
3. Solvents such as chloroform- d , benzene- d_6 , and toluene- d_8 , also remove residual water azeotropically.

How to Avoid TMS Evaporation

1. Extended storage of TMS-containing solvents can lead to some loss of TMS. Storing these solvents in Sure/Seal™ bottles virtually eliminates such a loss.*
2. Purchase TMS-containing solvents in single-use ampules.

** To dispense the product from Sure/Seal bottle or septum vials, use standard syringe needle techniques.*

We recommend ampules for customers concerned with maintaining high product integrity because once a solvent bottle is opened, moisture absorption and proton exchange with the atmosphere can occur rapidly.

For details and recommended procedures, refer to Aldrich Technical Bulletin AL-134 at

Aldrich.com/technicalbulletins



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