

CIL

Cambridge Isotope Laboratories, Inc.  
[www.isotope.com](http://www.isotope.com)

NMR SOLVENTS

# Deuterated Solvents for NMR

- NMR Solvents
- NMR Reference Standards
- NMR Tubes



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## CONTACT INFORMATION

### CONTACT CIL BY PHONE, FAX OR E-MAIL

The CIL Customer Service Department is open Monday-Thursday 8:00 A.M. to 5:30 P.M.; Friday 8:00 A.M. to 5:00 P.M. EST.

Phone	Fax	E-mail
1-800-322-1174 (USA)	1-978-749-2768	cilsales@isotope.com (North America)
1-800-643-7239 (Canada)		intlsales@isotope.com (International)
1-978-749-8000 (International)		envsales@isotope.com (Environmental Products)
1-800-322-1174 (Environmental)		
1-800-ISOTOPE ( US Regional Sales Manager)		

### CONTACT YOUR REGIONAL SALES MANAGER

Please contact your local sales representative to request a quote or discuss long term blanket discount orders. Dialing 1-800-ISOTOPE within the US will automatically put you in touch with your local Sales Manager. You may also visit our Web site at [www.isotope.com](http://www.isotope.com) for a list of Regional Sales Managers and the areas they service.

### CONTACT YOUR CUSTOMER ACCOUNT COORDINATOR

In order to provide our loyal customers with seamless customer service, each Regional Sales Manager has a dedicated Customer Account Coordinator assigned to their territory. Your Customer Account Coordinator is available to process your orders and quote requests as well as to confirm the delivery status of your order. Please contact your local Customer Account Coordinator to request a quote or to place an order. For a listing of Domestic and International Customer Account Coordinators and the areas they service, please visit our Web site at [www.isotope.com](http://www.isotope.com).

### CONTACT YOUR INTERNATIONAL DISTRIBUTOR

In order to provide our international customers with the best service possible, CIL has an established network of independent international distributors. Most of our distributors have worked with CIL for more than ten years. To request a quotation or place an order, please contact your local distributor noted on back cover. Our International Customer Service Department is also available to assist you.

## SHIPPING INFORMATION

Shipments within the United States will be sent via UPS, Federal Express, or truck. Canadian shipments will be sent via Federal Express or truck.

- International shipments of non-hazardous materials will be sent via Federal Express or best method.
- Hazardous materials will be shipped by air freight, surface vessel or Federal Express where applicable. CIL tries to be as cost effective as possible, but the carrier may place additional charges.
- Hazardous substances are identified with the appropriate UN number and transported in compliance with UN recommendations.
- We will oblige your shipping instructions whenever it is feasible to do so. CIL reserves the right to change the method of transportation if required to comply with transportation regulations. Such a change would not alter your responsibility for payment of shipping charges. Additional shipping charges may apply.

## CATALOG LISTINGS INCLUDE

New Indicator: **NEW**

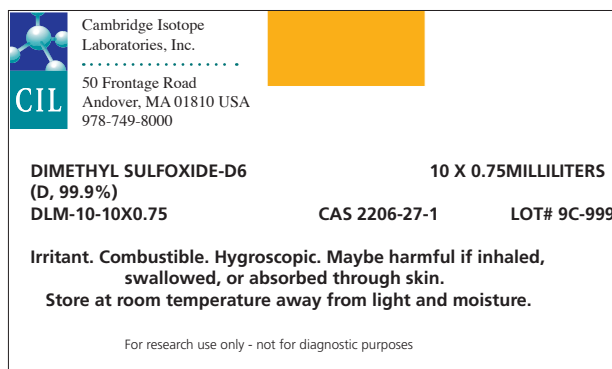
Compound Name	Enrichment	Alternative Name	Formula	Density	Molecular Weight *	Unit
<b>Dimethyl Sulfoxide-d<sub>6</sub></b>	(D,99.9%)	(contains 0.05% v/v TMS)	(DMSO)			
CIL Catalog # — DLM-10tb			CD <sub>3</sub> SOCD <sub>3</sub>	mw 84.17		10x0.6 mL
CAS # — [2206-27-1]				d 1.18		10x0.75 mL
						10x1 g
						3x(10x1 g)
						5 g
						10 g
						10x10 g
						3x(10x10 g)
						25 g
						50 g

\* Molecular weight is based on 100% enrichment

\*\* Stable if stored under normal conditions, unless otherwise noted

## OUR LABELS INCLUDE

- Product name and description
- Health and safety information
- Lot specific number
- Package size
- Pictograms for hazard recognition
- CAS numbers
- Storage information
- Packaging number
- Catalog number



## TECH INFO:

Each batch of CIL solvent is routinely tested for chemical and isotopic purity after initial purification, before packaging, and after packaging.

## HAZARDOUS ICONS



Biohazard



Corrosive

Environmental  
Danger

Explosive



Flammable



Harmful Irritant

















Oxidizing



Toxic

Compounds listed in this catalog are considered non-hazardous unless otherwise noted.

				unit
<b>Acetic Acid-d<sub>4</sub></b> (D,99.5%)				
DLM-12 [1186-52-3] UN# 2789	CD <sub>3</sub> COOD	mw 64.08 d 1.12	10 g 25 g 50 g	
				
<b>Acetic Acid-d<sub>4</sub> "100%"</b> (D,99.93%)				
DLM-41 [1186-52-3] UN# 2789	CD <sub>3</sub> COOD	mw 64.08 d 1.12	10x0.75 mL 5 mL	
				
<b>Acetone-d<sub>6</sub></b> (D,99.9%)				
DLM-9 [666-52-4] UN# 1090	CD <sub>3</sub> COCD <sub>3</sub>	mw 64.12 d 0.87	10x0.6 mL 10x0.75 mL 5x3 mL 1 L 10x1 g 3x(10x1 g) 10 g 10x10 g 3x(10x10 g) 25 g	
 				
<b>Acetone-d<sub>6</sub></b> (D,99.9%) (contains 1% v/v TMS)				
DLM-9ta [666-52-4] UN# 1090	CD <sub>3</sub> COCD <sub>3</sub>	mw 64.12 d 0.87	10x1 g 3x(10x1 g) 10 g 10x10 g 3x(10x10 g) 25 g	
 				
<b>Acetone-d<sub>6</sub></b> (D,99.9%) (contains 0.05% v/v TMS)				
DLM-9tb [666-52-4] UN# 1090	CD <sub>3</sub> COCD <sub>3</sub>	mw 64.12 d 0.87	10x1 g 3x(10x1 g) 10 g 10x10 g 3x(10x10 g) 25 g	
 				
<b>Acetone-d<sub>6</sub> "100%"</b> (D,99.96%)				
DLM-38 [666-52-4] UN# 1090	CD <sub>3</sub> COCD <sub>3</sub>	mw 64.12 d 0.87	5x0.5 mL 10x0.5 mL 10x0.6 mL 5x0.75 mL 10x0.75 mL 5 mL	
 				
<b>Acetone-d<sub>6</sub> "100%"</b> (D,99.96%) (contains 0.03% v/v TMS)				
DLM-38tc [666-52-4] UN# 1090	CD <sub>3</sub> COCD <sub>3</sub>	mw 64.12 d 0.87	10x0.75 mL	
 				
<b>Acetonitrile-d<sub>3</sub> HPLC grade</b> (D,96-97%)				
DLM-20 [2206-26-0] UN# 1648	(contains approximately 15-20% D <sub>2</sub> O) CD <sub>3</sub> C=N	mw 44.07 d 0.84	1 L	
 				

unit

**Acetonitrile-d<sub>3</sub>** (D,96-97%)

DLM-22 [2206-26-0] UN# 1648	CD <sub>3</sub> C=N	mw 44.07 d 0.84	1 L
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**Acetonitrile-d<sub>3</sub>** (D,99.8%)

DLM-21 [2206-26-0] UN# 1648	CD <sub>3</sub> C=N	mw 44.07 d 0.84	10x0.6 mL 10x0.75 mL 1 L 10x1 g 3x(10x1 g) 10 g 25 g 50 g
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**Acetonitrile-d<sub>3</sub>** (D,99.8%) (contains 0.05% v/v TMS)

DLM-21tb [2206-26-0] UN# 1648	CD <sub>3</sub> C=N	mw 44.07 d 0.84	10x0.6 mL
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**Acetonitrile-d<sub>3</sub> "100%"** (D,99.96%)

DLM-53 [2206-26-0] UN# 1648	CD <sub>3</sub> C=N	mw 44.07 d 0.84	10x0.5 mL 10x0.6 mL 5x0.75 mL 10x0.75 mL 5 mL
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**Benzene-d<sub>6</sub>** (D,99.5%)

DLM-1 [1076-43-3] UN# 1114	C <sub>6</sub> D <sub>6</sub>	mw 84.15 d 0.95	10x0.6 mL 10x0.75 mL 10x1 g 3x(10x1 g) 5 g 10 g 10x10 g 25 g 50 g 100 g
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**Benzene-d<sub>6</sub>** (D,99.5%) (contains 0.05% v/v TMS)

DLM-1tb [1076-43-3] UN# 1114	C <sub>6</sub> D <sub>6</sub>	mw 84.15 d 0.95	10x0.6 mL <b>NEW</b> 10 g
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**Benzene-d<sub>6</sub> "100%"** (D,99.96%)










DLM-40 [1076-43-3] UN# 1114	C <sub>6</sub> D <sub>6</sub>	mw 84.15 d 0.95	5x0.5 mL 10x0.5 mL 5x0.75 mL <b>NEW</b> 10x0.6 mL 10x0.75 mL 5 mL
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**Benzene-d<sub>6</sub> "100%"** (D,99.96%) (contains 0.03% v/v TMS)



DLM-40tc [1076-43-3] UN# 1114	C <sub>6</sub> D <sub>6</sub>	mw 84.15 d 1.52	10x0.75 mL
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				unit
<b>Bromobenzene-d<sub>5</sub></b> (D,99%)				
DLM-398 [4165-57-5] UN# 2514		C <sub>6</sub> D <sub>5</sub> Br	mw 162.04 d 1.52	5 g 10 g 25 g
				
<b>Chlorobenzene-d<sub>5</sub></b> (D,99%)				
DLM-263 [3114-55-4] UN# 1134		C <sub>6</sub> D <sub>5</sub> Cl	mw 117.59 d 1.16	1 g 5 g
				
<b>Chloroform-d</b> (D,99.8%)				
DLM-7 [865-49-6] UN# 1888	No stabilizers are used in this product.	CDCl <sub>3</sub>	mw 120.38 d 1.50	10x0.6 mL 10x0.75 mL 10x1 g 3x(10x1 g) 50 g 100 g 10x100 g 3x(10x100 g)
				
<b>Chloroform-d</b> (D,99.8% stabilized with silver foil)				
DLM-7-50S DLM-7-100S [865-49-6]		CDCl <sub>3</sub>	mw 120.38 d 1.50	50 g 100 g
				
<b>Chloroform-d</b> (D,99.8%) (contains 1% v/v TMS)				
DLM-7ta [865-49-6] UN# 1888	No stabilizers are used in this product.	CDCl <sub>3</sub>	mw 120.38 d 1.50	10x1 g 3x(10x1 g) 50 g 100 g 10x100 g 3x(10x100 g)
				
<b>Chloroform-d</b> (D,99.8%) (contains 0.05% v/v TMS)				
DLM-7tb [865-49-6] UN# 1888	No stabilizers are used in this product.	CDCl <sub>3</sub>	mw 120.38 d 1.50	10x1 g 3x(10x1 g) 50 g 100 g 10x100 g 3x(10x100 g)
				
<b>Chloroform-d "100%"</b> (D,99.96%)				
DLM-29 [865-49-6] UN# 1888	No stabilizers are used in this product.	CDCl <sub>3</sub>	mw 120.38 d 1.50	10x0.25 mL 10x0.5 mL 10x0.6 mL 5x0.75 mL 10x0.75 mL 10 mL 5x10 mL 50 g
				
<b>Chloroform-d "100%"</b> (D,99.96%) (contains 0.03% v/v TMS)				
DLM-29tc [865-49-6] UN# 1888	No stabilizers are used in this product.	CDCl <sub>3</sub>	mw 120.38 d 1.50	10x0.75mL
				

				unit
<b>Cyclohexane-d<sub>12</sub></b> (D,99.5%)				
DLM-17 [1735-17-7] UN# 1145		C <sub>6</sub> D <sub>12</sub>	mw 96.23 d 0.89	5x1 g 10x1 g 3x(10x1 g) 5 g 10 g
 				
<b>Decalin-d<sub>18</sub></b> (D,99%) (Decahydronaphthalene)				
DLM-1386 [28788-42-3]	(cis/trans mixture)	C <sub>10</sub> D <sub>18</sub>	mw 156.36 d 0.896	1 g 5 g
 				
<b>trans-Decalin-d<sub>18</sub></b> (D,98%)				
DLM-1843 [493-02-7]		C <sub>10</sub> D <sub>18</sub>	mw 156.36 d 0.87	5 g
<b>Deuterium Bromide</b> (D,99%)				
DLM-3021 [13536-59-9]	(DBr 48% w/w solution in D <sub>2</sub> O)	DBr	mw 81.92 d 1.537	10 g (of soln.) 50 g (of soln.)
  <i>Packaged in clear glass ampoules only</i>				
<b>Deuterium Chloride</b> (D,99.5%)				
DLM-2 [7698-05-7]	(DCI 20% w/w solution in D <sub>2</sub> O)	DCI	mw 37.47 d 1.20	50 g (of soln.)
 <i>Packaged in clear glass ampoules only</i>				
<b>Deuterium Chloride "100%"</b> (D,99.96%)				
DLM-54 [7698-05-7]	(DCI 20% w/w solution in D <sub>2</sub> O)	DCI	mw 37.47 d 1.30	5 g (of soln.) 25 g (of soln.)
 <i>Packaged in clear glass ampoules only</i>				
<b>Deuterium Chloride</b> (D,99.5%)				
DLM-3 [7698-05-7]	(DCI 35% w/w solution in D <sub>2</sub> O)	DCI	mw 37.47 d 1.25	50 g (of soln.)
 <i>Packaged in clear glass ampoules only</i>				
<b>Deuterium Oxide</b> (D,70%)				
DLM-4-70 [7789-20-0] UN# 1957		D <sub>2</sub> O	mw 20.03 d 1.11	1 kg
<b>Deuterium Oxide</b> (D,70%) (sterility tested)				
DLM-2259-70 [7789-20-0] UN# 1957		D <sub>2</sub> O	mw 20.03 d 1.11	1 kg
<b>Deuterium Oxide</b> (D,99%)				
DLM-4-99 [7789-20-0] UN# 1957		D <sub>2</sub> O	mw 20.03 d 1.11	1 kg 5 kg
<b>Deuterium Oxide</b> (D,99.8%)				
DLM-4-99.8 [7789-20-0] UN# 1957		D <sub>2</sub> O	mw 20.03 d 1.11	1 kg



			unit
<b>Deuterium Oxide (D,99.8%) (sterility tested)</b>			
DLM-2259 [7789-20-0] UN# 1957	D <sub>2</sub> O	mw 20.03 d 1.11	<b>NEW</b> 100 mL 250 mL 1 L
<b>Deuterium Oxide (D,99.9%)</b>			
DLM-4 [7789-20-0] UN# 1957	D <sub>2</sub> O	mw 20.03 d 1.11	25 g 100 g 5x100 g 10x100 g 1000 g 1 L Inquire
<b>Deuterium Oxide (D,99.9%) (glass distilled, low paramagnetic, low conductivity)</b>			
DLM-11 [7789-20-0] UN# 1957	D <sub>2</sub> O	mw 20.03 d 1.11	100 g
<i>Packaged in plastic bottles only</i>			
<b>Deuterium Oxide "100%" (D,99.96%)</b>			
DLM-6 [7789-20-0] UN# 1957	D <sub>2</sub> O	mw 20.03 d 1.11	10x0.6 mL 5x0.7 mL 10x0.7 mL 5x(10x0.7 mL) 10x1 g 1000 g
<b>Deuterium Oxide "100%" (D,99.96%)</b>			
DLM-6-s [7789-20-0] UN# 1957	D <sub>2</sub> O	mw 20.03 d 1.11	10 g 50 g
<i>Packaged in serum bottles with Teflon coated rubber septum tops</i>			
<b>Deuterium Oxide "100%" (D,99.96%) (contains 0.01 mg/mL DSS)</b>			
DLM-6DB [7789-20-0] UN# 1957	D <sub>2</sub> O	mw 20.03 d 1.11	10x0.7 mL
<b>Deuterium Oxide "100%" (D,99.96%) (highest purity, glass distilled, low paramagnetic, low conductivity)</b>			
DLM-1172 [7789-20-0] UN# 1957	D <sub>2</sub> O	mw 20.03 d 1.11	10 g
<i>Packaged in plastic bottles only</i>			
<b>1,2-Dibromoethane-d<sub>4</sub> (D,99%)</b>			
DLM-195 [22581-63-1] UN# 1605	Br(CD <sub>2</sub> ) <sub>2</sub> Br	mw 191.87 d 2.20	10 g 25 g
			
<b>1,2-Dichlorobenzene-d<sub>4</sub> (D,99%)</b>			
DLM-158 [2199-69-1] UN# 1591	C <sub>6</sub> D <sub>4</sub> Cl <sub>2</sub>	mw 151.03 d 1.30	1 g 5 g
			
<b>1,2-Dichloroethane-d<sub>4</sub> (D,99%)</b>			
DLM-18 [17060-07-0] UN# 1184	Cl(CD <sub>2</sub> ) <sub>2</sub> Cl	mw 102.98 d 1.30	1 g 5x1 g 5 g

			unit
<b>Diethyl Ether-d<sub>10</sub></b> (D,99%)			
DLM-1592 [2679-89-2] UN# 1155	(CD <sub>3</sub> CD <sub>2</sub> ) <sub>2</sub> O	mw 84.18 d 0.82	1 g 5x1 g 5 g
	Packaged in ampoules only		
<b>Diglyme-d<sub>14</sub></b> (D,98%)			
DLM-47 [38086-00-9]	(CD <sub>3</sub> OCD <sub>2</sub> CD <sub>2</sub> ) <sub>2</sub> O	mw 148.26 d 1.035	Please inquire
<b>N,N-Dimethylformamide-d<sub>7</sub></b> (D,99.5%) (DMF)			
DLM-25 [4472-41-7]	DCON(CD <sub>3</sub> ) <sub>2</sub>	mw 80.14 d 1.04	5x1 g 10x1 g 5 g 10 g
	Packaged in ampoules only		
<b>N,N-Dimethylformamide-d<sub>7</sub></b> (D,99.5%) (contains 0.05% v/v TMS) (DMF)			
DLM-25tb [4472-41-7]	DCON(CD <sub>3</sub> ) <sub>2</sub>	mw 80.14 d 1.04	10x0.6 mL
	Packaged in ampoules only		
<b>Dimethyl Sulfoxide-d<sub>6</sub></b> (D,99.9%) (DMSO)			
DLM-10 [2206-27-1]	CD <sub>3</sub> SOCD <sub>3</sub>	mw 84.17 d 1.18	10x0.6 mL 10x0.75 mL 5x3 mL 10x1 g 3x(10x1 g) 5 g 10 g 10x10 g 3x(10x10 g) 25 g 50 g <b>NEW</b> 1000 g
<b>Dimethyl Sulfoxide-d<sub>6</sub></b> (D,99.9%) (DMSO)			
DLM-10-s [2206-27-1]	CD <sub>3</sub> SOCD <sub>3</sub>	mw 84.17 d 1.18	10 g 25 g
	Packaged in serum bottles with Teflon coated rubber septum tops		
<b>Dimethyl Sulfoxide-d<sub>6</sub></b> (D,99.9%) (contains 1% v/v TMS) (DMSO)			
DLM-10ta [2206-27-1]	CD <sub>3</sub> SOCD <sub>3</sub>	mw 84.17 d 1.18	10x1 g 3x(10x1 g) 5 g 10 g 10x10 g 3x(10x10 g) 25 g 50 g
<b>Dimethyl Sulfoxide-d<sub>6</sub></b> (D,99.9%) (contains 0.05% v/v TMS) (DMSO)			
DLM-10tb [2206-27-1]	CD <sub>3</sub> SOCD <sub>3</sub>	mw 84.17 d 1.18	10x0.6 mL 10x0.75 mL 10x1 g 3x(10x1 g) 5 g 10 g 10x10 g 3x(10x10 g) 25 g 50 g

unit

**Dimethyl Sulfoxide-d<sub>6</sub> "100%"** (D,99.96%) (DMSO)

DLM-34 [2206-27-1]	CD <sub>3</sub> SOCD <sub>3</sub>	mw 84.17 d 1.18	10x0.25 mL 5x0.5 mL 10x0.5 mL 10x0.6 mL 5x0.75 mL 10x0.75 mL 5 mL
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**Dimethyl Sulfoxide-d<sub>6</sub> "100%"** (D,99.96%) (contains 0.03% v/v TMS) (DMSO)

DLM-34tc [2206-27-1]	CD <sub>3</sub> SOCD <sub>3</sub>	mw 84.17 d 1.18	10x0.75 mL
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**1,4-Dioxane-d<sub>8</sub>** (D,99%) (*p*-Dioxane)

DLM-28 [17647-74-4]	C <sub>4</sub> D <sub>8</sub> O <sub>2</sub>	mw 96.15 d 1.13	5x1 g 10x1 g 3x(10x1 g) 5 g 10 g 25 g
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UN# 1165

**DSS — D<sub>2</sub>O reference standard** (Sodium 2,2-Dimethyl-2-Silapentane-5-Sulfonate)

DLM-32 [2039-96-5]	Chemical Purity: 97% (CH <sub>3</sub> ) <sub>2</sub> Si(CH <sub>2</sub> ) <sub>3</sub> SO <sub>3</sub> Na	mw 218.31	1 g 10 g 50 g
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UN# 1165

**Ethanol-d** (D,99%) (Contains ≤ 6% D<sub>2</sub>O) (Ethyl Alcohol)

DLM-16 [925-93-9]	CH <sub>3</sub> CH <sub>2</sub> OD	mw 47.08 d 0.89	50 g 2x50 g
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UN# 1170

**Ethanol-d<sub>6</sub>** (D,99%) (anhydrous) (Ethyl Alcohol)

DLM-31 [1516-08-1]	CD <sub>3</sub> CD <sub>2</sub> OD	mw 52.11 d 0.89	5x1 g 10x1 g 5 g
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Packaged in ampoules only

**Ethanol-d<sub>6</sub>** (D,99%) (Contains ≤ 6% D<sub>2</sub>O) (Ethyl Alcohol)

DLM-31B [1516-08-1]	CD <sub>3</sub> CD <sub>2</sub> OD	mw 52.11 d 0.89	5x1 g 5 g
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**Ethylene Glycol-d<sub>6</sub>** (D,98%)

DLM-132 [107-21-1]	DOCD <sub>2</sub> CD <sub>2</sub> OD	mw 68.11 d 1.113	5 g
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**Fluorobenzene-d<sub>5</sub>** (D,98%)

DLM-617 [1423-10-5]	C <sub>6</sub> D <sub>5</sub> F	mw 101.13 d 1.08	1 g
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UN# 2387

**n-Heptane-d<sub>16</sub>** (D,98%)

DLM-423 [33838-52-7]	CD <sub>3</sub> (CD <sub>2</sub> ) <sub>5</sub> CD <sub>3</sub>	mw 116.30 d 0.794	1 g 5 g
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UN# 1206

unit

**Hexafluoroacetone Trideuterate (D,99.5%)**

DLM-1020 [109640-39-3]	$\text{CF}_3\text{COCF}_3 \cdot 3 \text{D}_2\text{O}$	mw 226.11 d 1.71	10 g
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**1,1,1,3,3,3-Hexafluoroisopropanol-d<sub>2</sub> (D,98%) (Hexafluoroisopropyl Alcohol, HFIP)**

DLM-143 [38701-74-5]	$(\text{CF}_3)_2\text{CDOD}$	mw 170.05 d 1.60	1 g 5x1 g 5 g 10 g
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**n-Hexane-d<sub>14</sub> (D,98%)**

DLM-139 [21666-38-6]	$\text{CD}_3(\text{CD}_2)_4\text{CD}_3$	mw 100.26 d 0.767	1 g 5 g
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UN# 1208

**Isopropanol-d<sub>8</sub> (D,99%) (2-Propyl Alcohol)**

DLM-44 [22739-76-0]	$(\text{CD}_3)_2\text{CDOD}$	mw 68.14 d 0.90	5 g 25 g
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UN# 1219

**Lithium Deuterioxide (D,99.5%)**

DLM-2173 [12159-20-5]	(3N in D <sub>2</sub> O solution) $\text{LiOD}$	mw 24.96 d 1.218	25 g 100 g
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Packaged in plastic bottles only

**Methanol-d (D,99%) (Methyl Alcohol)**

DLM-15 [1455-13-6]	$\text{CH}_3\text{OD}$	mw 33.05 d 0.81	50 g 2x50 g
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UN# 1230

**Methanol-d<sub>4</sub> (D,99.8%) (Methyl Alcohol)**

DLM-24 [811-98-3]	$\text{CD}_3\text{OD}$	mw 36.07 d 0.89	10x0.6 mL 10x0.75 mL 1 L 10x1 g 3x(10x1 g) 5 g 10 g 10x10 g 25 g 50 g
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UN# 1230

**Methanol-d<sub>4</sub> (D,99.8%) (Methyl Alcohol)**

DLM-24-s [811-98-3]	$\text{CD}_3\text{OD}$	mw 36.07 d 0.89	10 g 25 g 50 g
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UN# 1230



Packaged in serum bottles with Teflon coated rubber septum tops

**Methanol-d<sub>4</sub> (D,99.8%) (contains 0.05% v/v TMS) (Methyl Alcohol)**

DLM-24tb [811-98-3]	$\text{CD}_3\text{OD}$	mw 36.07 d 0.89	10x0.6 mL 10x0.75 mL 10x1 g 10 g 10x10 g
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UN# 1230



unit

**Methanol-d<sub>4</sub> "100%"** (D,99.95%) (Methyl Alcohol)

DLM-51 [811-98-3]	CD <sub>3</sub> OD	mw 36.07 d 0.89	10x0.25 mL 5x0.5 mL 10x0.5 mL 10x0.6 mL 5x0.75 mL 10x0.75 mL
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UN# 1230

**Methylcyclohexane-d<sub>14</sub>** (D,99.5%)

DLM-288 [10120-28-2]	C <sub>6</sub> D <sub>11</sub> CD <sub>3</sub>	mw 112.27 d 0.88	1 g 5 g
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UN# 2296

**Methylene Chloride-d<sub>2</sub>** (D,99.9%) (Dichloromethane)

DLM-23 [1665-00-5]	CD <sub>2</sub> Cl <sub>2</sub>	mw 86.95 d 1.35	10x0.75 mL 5x3 mL 5x1 g 10x1 g 3x(10x1 g) 5 g 10 g 25 g
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UN# 1593

**Methylene Chloride-d<sub>2</sub>** (D,99.9%) (contains 0.05% v/v TMS) (Dichloromethane)

DLM-23tb [1665-00-5]	CD <sub>2</sub> Cl <sub>2</sub>	mw 86.95 d 1.35	10x0.6 mL
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UN# 1593

**Methylene Chloride-d<sub>2</sub> "100%"** (D,99.96%) (Dichloromethane)

DLM-55 [1665-00-5]	CD <sub>2</sub> Cl <sub>2</sub>	mw 86.95 d 1.35	10x0.5 mL 10x0.6 mL 5x0.75 mL 10x0.75 mL 5 mL
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UN# 1593

**N-Methyl-2-pyrrolidinone-d<sub>9</sub>** (D,97%-99%) (NMP)DLM-1988-97  
[185964-60-7]mw 108.19  
d 1.026 Please inquire**Nitric Acid-d** (D,99%)

DLM-3037 [13587-52-5]	(65-70% w/w solution in D <sub>2</sub> O)	DNO <sub>3</sub>	mw 64.02 d 1.026	5 g (of soln.) 25 g (of soln.)
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Packaged in clear glass ampoules only

**Nitrobenzene-d<sub>5</sub>** (D,99%)

DLM-294 [4165-60-0]	C <sub>6</sub> D <sub>5</sub> NO <sub>2</sub>	mw 128.14 d 1.25	5 g 10 g 25 g
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UN# 1662

**Nitromethane-d<sub>3</sub>** (D,99%)

DLM-30 [13031-32-8]	CD <sub>3</sub> NO <sub>2</sub>	mw 64.06 d 1.20	10 g 25 g
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UN# 1261



unit

**n-Octane-d<sub>18</sub>** (D,99%)

DLM-50 [17252-77-6]		$\text{CD}_3(\text{CD}_2)_6\text{CD}_3$	mw 132.34 d 0.815	1 g 5 g
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UN# 1262

**n-Pentane-d<sub>12</sub>** (D,98%)

DLM-1213 [2031-90-5]		$\text{CD}_3(\text{CD}_2)_3\text{CD}_3$	mw 84.22 d 0.73	1 g 5 g
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UN# 1265

**Phosphoric Acid-d<sub>3</sub>** (D,99%)

DLM-1132 [14335-33-2]	(approximately 85% w/w solution in D <sub>2</sub> O)	$\text{D}_3\text{PO}_4$	mw 101.01 d 1.74	50 g 100 g
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**Pyridine-d<sub>5</sub>** (D,99.5%)

DLM-13 [7291-22-7]		$\text{C}_5\text{D}_5\text{N}$	mw 84.13 d 1.05	5x1 g 10x1 g 3x(10x1 g) 10 g 25 g 50 g
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UN# 1282

**Pyridine-d<sub>5</sub>** (D,99.5%) (contains 0.05% v/v TMS)

DLM-13tb [7291-22-7]		$\text{C}_5\text{D}_5\text{N}$	mw 84.13 d 1.05	10x0.6 mL 5x1 g 10x1 g 3x(10x1 g) 10 g 25 g 50 g
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UN# 1282

**Pyridine-d<sub>5</sub> "100%"** (D,99.94%)

DLM-39 [7291-22-7]		$\text{C}_5\text{D}_5\text{N}$	mw 84.13 d 1.05	5x0.5 mL 10x0.5 mL 5x0.75 mL 10x0.75 mL 5 mL
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UN# 1282

**Sodium Deuterioxide** (D,99.5%)

DLM-57 [14014-06-3]	(NaOD 30% w/w solution in D <sub>2</sub> O)	$\text{NaOD}$	mw 41.00 d 1.46	50 g
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UN# 1282



Packaged in polyethylene bottles

**Sodium Deuterioxide** (D,99.5%)

DLM-45 [14014-06-3]	(NaOD 40% w/w solution in D <sub>2</sub> O)	$\text{NaOD}$	mw 41.00 d 1.46	50 g 100 g
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UN# 1282



Packaged in polyethylene bottles

**Sulfuric Acid-d<sub>2</sub>** (D,99%)

DLM-33 [13813-19-9]	(96-98% solution in D <sub>2</sub> O)	$\text{D}_2\text{SO}_4$	mw 100.09 d 1.86	50 g
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UN# 1282



Packaged in clear glass ampoules only

unit

**1,1,2,2-Tetrachloroethane-d<sub>2</sub>** (D,99.6%) (TCE)

DLM-35 [33685-54-0]	$\text{Cl}_2\text{CDCDCl}_2$	mw 169.86 d 1.62	5 g 10 g 100 g
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UN# 1702

**Tetrahydrofuran-d<sub>8</sub>** (D,99.5%) (THF)

DLM-36 [1693-74-9]	$\text{C}_4\text{D}_8\text{O}$	mw 80.16 d 0.99	10x0.75 mL 5x3 mL 5x1 g 10x1 g 3x(10x1 g) 5 g 10 g
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UN# 2056



Packaged in ampoules only

**Tetrahydrofuran-d<sub>8</sub> "100%"** (D,99.95%) (THF)

DLM-56 [1693-74-9]	$\text{C}_4\text{D}_8\text{O}$	mw 80.16 d 0.99	10x0.5 mL 10x0.75 mL 5 mL
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UN# 2056

**Tetramethylsilane** (TMS)

DLM-43 [75-76-3]	(NMR grade) Chemical Purity: 99.9%	$(\text{CH}_3)_4\text{Si}$	mw 88.22 d 0.64	50 g
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**TMSP-2,2,3,3-d<sub>4</sub>** (D,98%) (Sodium 3-Trimethylsilylpropionate)

DLM-48 [24493-21-8]	(D <sub>2</sub> O reference standard)	$(\text{CH}_3)_3\text{SiCD}_2\text{CD}_2\text{CO}_2\text{Na}$	mw 172.27 d 1.52	1 g 5x1 g 5 g
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**Toluene-d<sub>8</sub>** (D,99.5%)

DLM-5 [2037-26-5]	$\text{C}_6\text{D}_5\text{CD}_3$	mw 100.19 d 0.94	10x1 g 3x(10x1 g) 5 g 10 g 25 g
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UN# 1294

**Toluene-d<sub>8</sub> "100%"** (D,99.94%)

DLM-42 [2037-26-5]	$\text{C}_6\text{D}_5\text{CD}_3$	mw 100.19 d 0.94	5x0.5 mL 10x0.5 mL 5x0.75 mL 10x0.75 mL 5 mL
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UN# 1294

**Trifluoroacetic Acid-d** (D,99.5%)

DLM-46 [599-00-8]	$\text{CF}_3\text{COOD}$	mw 115.03 d 1.50	10x0.75 mL 10x1 g 10 g 25 g 4x25 g
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UN# 2699



Packaged in ampoules only

**2,2,2-Trifluoroethanol-d<sub>2</sub>** (D,98%) (Trifluoroethyl Alcohol)

DLM-2318 [77253-67-9]	$\text{CF}_3\text{CD}_2\text{OH}$	mw 102.05 d 1.45	1 g 5 g
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unit

**2,2,2-Trifluoroethanol-d<sub>3</sub>** (D,99%) (Trifluoroethyl Alcohol)

DLM-27	CF <sub>3</sub> CD <sub>2</sub> OD	mw 103.06	1 g
[77253-67-9]		d 1.45	5x1 g

**2,2,2-Trifluoroethanol-d<sub>3</sub> "100%"** (D,99.85%) (Trifluoroethyl Alcohol)

DLM-58	CF <sub>3</sub> CD <sub>2</sub> OD	mw 103.06	1 g
[77253-67-9]		d 1.45	5 g

**Water, Deuterium Depleted**

DLM-52	(2-3 ppm Deuterium)	H <sub>2</sub> O	mw 18.02	25 g
[7732-18-5]			d 1.00	100 g

**NEW 1,3,5-Trimethyl Benzene** (D<sub>1,2</sub>, 98%) (Mesitylene)

DLM-3105	C <sub>6</sub> D <sub>3</sub> (CD <sub>3</sub> ) <sub>3</sub>	mw 132.26	5 g
[69441-16-3]			

UN# 2325

**o-Xylene-d<sub>10</sub>** (D,98%)

DLM-808	C <sub>6</sub> D <sub>4</sub> (CD <sub>3</sub> ) <sub>2</sub>	mw 116.23	5 g
[56004-61-6]		d 0.953	

UN# 1307

**p-Xylene-d<sub>10</sub>** (D,98%)

DLM-313	C <sub>6</sub> D <sub>4</sub> (CD <sub>3</sub> ) <sub>2</sub>	mw 116.23	5 g
[41051-88-1]		d 0.948	

UN# 1307

**CARBON-12 AND CARBON-12/DEUTERIUM LABELED SOLVENTS (Carbon-13 Depleted)****Benzene** (<sup>12</sup>C<sub>6</sub>,99.95%)

CLM-867	( <sup>13</sup> C depleted)	*C <sub>6</sub> H <sub>6</sub>	mw 78.05	0.8 mL
[71-43-2]				

**Chloroform** (<sup>12</sup>C,99.95%;D,99%)

CDLM-844	( <sup>13</sup> C depleted)	*CDCl <sub>3</sub>	mw 120.38	Please inquire
[865-49-6]				

**Methanol** (<sup>12</sup>C,99.95%) (Methyl Alcohol)

CLM-2472	( <sup>13</sup> C depleted)	*CH <sub>3</sub> OH	mw 32.04	1g
[67-56-1]				

**Methanol** (<sup>12</sup>C,99.95%;D<sub>4</sub>,99.5%) (Methyl Alcohol)

CDLM-01	( <sup>13</sup> C depleted)	*CD <sub>3</sub> OD	mw 36.07	0.8 mL
[811-98-3]				5 g

**NMR REFERENCE STANDARDS**

As the leading supplier of NMR reference standards to the world's largest NMR manufacturers, CIL has an extensive offering of NMR reference standards. Accompanied by a complete technical data package, these standards help to assure proper spectrometer performance. CIL's total quality assurance protocols and in-house manufacturing capabilities guarantee the highest standard of quality the first time and every time. These NMR Reference Standards have been evaluated and determined to meet or exceed industry requirements. A representative listing of these NMR Reference Standards is provided below. We also welcome your requests for custom formulations of other reference standards as well as alternate fill heights of existing reference standards. Please contact us if you require a reference standard that is not listed below. CIL routinely produces other reference standards which are generally available from stock.

**1% 1,2-Dichlorobenzene in Acetone-d<sub>6</sub>** (99.9%D)

DLM-79	Application: <sup>1</sup> H-Resolution	5mm x 8"
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**0.1% Ethylbenzene+ 0.01% TMS in Chloroform-d "100%"** (99.96%D)

DLM-74	Application: <sup>1</sup> H-Sensitivity	5mm x 8"
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unit

**1% 3-Heptanone in Chloroform-d (99.8%D)**DLM-67 Application: <sup>1</sup>H APT Test 5mm x 8"**12% TMS in Chloroform**ULM-73 Application: <sup>1</sup>H-Reference/Calibration 5mm x 8"**5% Ethylbenzene+ 2% TMS in Chloroform-d (99.8%D)**DLM-84 Application: <sup>1</sup>H-Sensitivity/Reference 5mm x 8"**1% Chloroform in Acetone-d<sub>6</sub> (99.9%D)**DLM-76 Application: <sup>1</sup>H-Line Shape 5mm x 8"**0.1 mg/mL GdCl<sub>3</sub> • 6H<sub>2</sub>O in D<sub>2</sub>O (99.96%D)**DLM-90 Application: <sup>1</sup>H-Homogeneity 5mm x 8"**40% p-Dioxane in Benzene-d<sub>6</sub> (99.6%D)**DLM-72 Application: <sup>13</sup>C-Sensitivity/Resolution 5mm x 8"**30% Menthol (by weight) in Chloroform-d (99.8%D)**DLM-66 Application: <sup>13</sup>C App Test 5mm x 8"**90% Formamide in DMSO-d<sub>6</sub> (99.9%D)**DLM-68 Application: <sup>15</sup>N-Sensitivity 5mm x 8"**0.0485 M Triphenylphosphate in Chloroform-d (99.8%D)**DLM-77 Application: <sup>31</sup>P-Sensitivity 5mm x 8"**0.05% α,α,α,-Trifluorotoluene in Benzene-d<sub>6</sub> (99.6%D)**DLM-78 Application: <sup>19</sup>F-Sensitivity 5mm x 8"**0.1% Methanol-<sup>13</sup>C+0.3 mg/mL GdCl<sub>3</sub> in 98.9% D<sub>2</sub>O+1% H<sub>2</sub>O**

CDLM-100 Application: Auto Test Sample 5mm x 8"

**0.1 mg/mL GdCl<sub>3</sub>+0.1% DSS in 20% H<sub>2</sub>O in D<sub>2</sub>O**

DLM-88 Application: Gradient Shimming 5mm x 8"

**1% <sup>13</sup>CH<sub>3</sub>I, 0.2% Cr(acac)<sub>3</sub>+ 1% (CH<sub>3</sub>O)<sub>3</sub>P in CDCl<sub>3</sub> "100%"**

CDLM-96 Application: Indirect Detection Test 5mm x 8"

**0.2% Cr(acac)<sub>3</sub>+ 2% Benzamide (<sup>15</sup>N,98%+) in DMSO-d<sub>6</sub> "100%" (99.96%D)**

DNLM-97 Application: Indirect Detection Test 5mm x 8"

**100% Ethylene Glycol**

ULM-71 Application: High Temperature Calibrant 5mm x 8"

**100% Methanol**

ULM-69 Application: Low Temperature Calibrant 5mm x 8"

**10% TMS in Methanol**

ULM-92 Application: Low Temperature Measurement 5mm x 8"

**NEW 0.1M Urea-<sup>15</sup>N+0.1M MeOH-<sup>13</sup>C in DMSO-d<sub>6</sub> 100%**

CDNLM-5003 Application: Indirect Detection Experiments 5mm x 8"

**50mM Sodium Acetate +1% Water in Deuterium Oxide**

DLM-5032-50mL Application: Homogeneity Standard Please inquire

**1% Water in Deuterium Oxide**

DLM-7005 Application: Homogeneity Standard Please inquire

Since 2006, CIL has partnered with Norell to offer our customers the convenience and quality of purchasing our solvents and Norell's standard and select series NMR tubes together. CIL offers Norell NMR tubes in North America only. International customers should contact their local independent distributor.

### **NORELL™ TUBES** (Sold only in North America)

#### **5 mm, 100 Mhz, 7" Standard Series**

502-7	NMR Tube	50 Pack
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#### **5 mm, 100 Mhz, 8" Standard Series**

502-8	NMR Tube	50 Pack
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#### **5 mm, 200 Mhz, 7" Select Series**

S-5-200-7	NMR Tube	5 Pack
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#### **5 mm, 200 Mhz, 8" Select Series**

S-5-200-8	NMR Tube	5 Pack
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#### **5 mm, 300 Mhz, 7" Select Series**

S-5-300-7	NMR Tube	5 Pack
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#### **5 mm, 300 Mhz, 7" Standard Series**

XR-55-7	NMR Tube	25 Pack
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#### **5 mm, 300 Mhz, 8" Select Series**

S-5-300-8	NMR Tube	5 Pack
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#### **5 mm, 300 Mhz, 8" Standard Series**

XR-55-8	NMR Tube	25 Pack
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#### **5 mm, 400 Mhz, 7" Select Series**

S-5-400-7	NMR Tube	5 Pack
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#### **5 mm, 400 Mhz, 7" Standard Series**

507-HP-7	NMR Tube	5 Pack
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#### **5 mm, 400 Mhz, 8" Select Series**

S-5-400-8	NMR Tube	5 Pack
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#### **5 mm, 400 Mhz, 8" Standard Series**

507-HP-8	NMR Tube	5 Pack
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#### **5 mm, 500 Mhz, 7" Select Series**

S-5-500-7	NMR Tube	5 Pack
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#### **5 mm, 500 Mhz, 7" Standard Series**

508-UP-7	NMR Tube	5 Pack
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#### **5 mm, 500 Mhz, 8" Select Series**

S-5-500-8	NMR Tube	5 Pack
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#### **5 mm, 500 Mhz, 8" Standard Series**

508-UP-8	NMR Tube	5 Pack
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#### **5 mm, 600 Mhz, 7" Select Series**

S-5-600-7	NMR Tube	5 Pack
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## USE AND HANDLING OF NMR SOLVENTS

CIL has implemented extensive quality control protocols for the evaluation of chemical and isotopic purities of our solvents. CIL understands that the increase in sensitivity and resolution of today's high field NMR instruments requires solvents with the highest chemical purity as well as high isotopic enrichment. Each lot of our NMR solvents receives thorough quality control testing before being released for shipment. All ampoules and bottles are clearly marked with both a production and a packaging lot number for easy tracking in the unlikely event that a problem should occur.

### WATER PEAKS

Water contamination is a common problem for deuterated NMR solvents. There are several things that can be done to minimize/eliminate water peaks.

- Consider using single-use ampoules. Many of our solvents are available in single-use breakseal ampoules ranging in size from 0.25 mL to 3 mL.
- Handle solvents in a dry atmosphere.
- Dry NMR tubes and pipettes used for sample preparation overnight in an oven and cool them in a desiccator prior to use.
- Precondition an NMR tube by rinsing it with D<sub>2</sub>O. Remove residual D<sub>2</sub>O by rinsing first with methanol-D<sub>4</sub> or acetone-D<sub>6</sub> and then with the solvent of choice. This process will not remove water, but it will exchange the protons for deuterium and minimize the water peak.

### "100%" D<sub>2</sub>O

To avoid loss of enrichment due to exchange with ambient moisture, "100%" D<sub>2</sub>O stored in a serum bottle should be sampled with a syringe that has been preflushed with dry nitrogen. Additionally, a volume of dry nitrogen equal to the amount of D<sub>2</sub>O being removed should be injected into the serum bottle prior to withdrawing D<sub>2</sub>O.

### TMS EVAPORATION

When stored at room temperature (unless noted below) and properly capped, solvents containing TMS should not suffer from TMS evaporation. However, upon extended storage of these solutions, some loss of TMS may occur.

### STORAGE

All serum bottles should be stored upright in the refrigerator; we do not recommend freezing. We also recommend that chloroform, diethyl ether, diglyme, tetrahydrofuran, and TMS be stored in the refrigerator.

## DEUTERATED CHLOROFORM

The deuterated chloroform produced at CIL is of the highest chemical purity. Over time chloroform will decompose regardless of the storage container or conditions. Over many months of storage at room temperature (for example, in a stockroom), deuterated chloroform can become acidic. However, decomposition is minimized if bottles are stored refrigerated in the dark.

CIL takes several precautions during production and packaging of chloroform-d to further minimize decomposition. Exposure to oxygen is minimized by using an argon atmosphere during production and packaging. Amber bottles are used to protect the product from light. Finally, silver foil is added to the solvent to act as a radical scavenger, which helps to stabilize the material over time.

### QUALITY CONTROL OF DEUTERATED CHLOROFORM

To ensure the highest quality, CIL routinely tests each batch of solvent for chemical and isotopic purity. The chemical purity is monitored during production and packaged using <sup>1</sup>H NMR, GC, Karl-Fisher titration for total water content and other wet chemical methods for acidity and various impurities.

### PROPER STORAGE AND USE OF DEUTERATED CHLOROFORM

Unopened bottles of chloroform-d should be refrigerated (-5°C to +5°C) to maximize shelf life. Moisture and oxygen will be introduced to the solvent following initial use through air entering the bottle upon opening. Decomposition can follow which results in the deuterated chloroform becoming acidic. The acidity can be easily tested using the following method:

#### TESTING DEUTERATED CHLOROFORM ACIDITY

A 1 mL aliquot of the solvent is added to a test tube containing 1 mL of distilled water (pH 5.0-7.0) and 2 drops of Bromothymol Blue (0.04% W/V). The color is compared to a 2 mL blank of distilled water (pH 5.0 – 7.0). If the sample solution is discolored (yellow) relative to the blank (blue-green), the deuterated chloroform is acidic.

Samples of deuterated chloroform which have become acidic can be easily neutralized using the following procedure:

- Place 3-5 grams of a 5Å molecular sieves into a 50 or 100g bottle of the solvent.
- Swirl slightly and allow to stand overnight. Excess water and traces of acidity will be removed. This is also the preferred way to store chloroform-d bottles once they have been opened, as it will keep the solvent dry and stable over time.
- Maintain an inert atmosphere (argon or nitrogen) in the bottle.
- Small "dust or powder" particles may break off from the molecular sieves. However, these particles can be removed simply by filtering the quantity of deuterated chloroform needed for an NMR sample through a small plug of glass wool or cotton in a glass pipette.

#### SPECIAL APPLICATIONS WHICH REQUIRE ULTRA DRY AND ACID FREE DEUTERATED CHLOROFORM

For applications involving highly acid-sensitive or moisture-sensitive compounds, deuterated chloroform can be purified further prior to use. Solvents treated in the following manner will be exceptionally dry and acid free.

- Place a glass wool plug into a disposable glass pipette (~7mm diameter).
- Add dry alumina powder into the pipette to a height of 3-4 cm.
- Pass the solvent through the small alumina bed into the sample container containing the product to be analyzed.
- Analyze the sample as soon as possible.

This procedure will ensure that the deuterated chloroform is dry and free of trace amounts of acid prior to contact with the sample. Note that the chloroform will react with basic compounds, such as alkaloids or amines. If the product is to be recovered, this should take place as soon as possible to minimize possible reaction.

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#### NMR SOLVENT TECHNICAL TIPS

- Often solvent users require a specific custom mixture of two or more solvents. CIL's expert packaging technicians are uniquely qualified to formulate custom solvent preparations.
- To measure acidity in deuterium oxide solutions: calculate pD by adding 0.4 to the reading taken from the glass electrode pH meter. (Glasoe and Long, J. Phys. Chem., 64, 188 (1960)).
- Dimethyl Sulfoxide (DMSO) has a melting point of 18°C, freezing close to room temperature. Sometimes when it is delivered it will be in a solid state. To return the material to a liquid state, thaw it in a warm water bath. Care must be taken to prevent water contamination.
- CIL recommends refrigeration of solvents packaged in septum bottles with the exception of DMSO-d<sub>6</sub> (18°C) to extend the product shelf life, high purity, and ensure product quality. Septum bottles should be tested after 6 months.
- In order to avoid isotopic contamination, some products, especially deuterated compounds, should be handled under an inert atmosphere, such as dry nitrogen or argon.
- CIL also specializes in <sup>13</sup>C depleted and deuterium depleted compounds. Please contact us if you do not see the <sup>13</sup>C depleted/ deuterium depleted compound of interest.
- We recommend that chloroform, diethyl ether, diglyme, tetrahydrofuran, and TMS be stored in the refrigerator.
- CIL welcomes your requests for custom formulations of reference standards not listed in this section.
- The NMR Solvent Data chart is available as a laminated reference document. Please contact your Customer Account Coordinator to request a copy.



Cambridge Isotope Laboratories, Inc.  
www.isotope.com

## NMR SOLVENTS

## NMR Solvent Data Chart

More Solvents, More Sizes, More Solutions

	<sup>1</sup> H Chemical Shift (ppm from TMS) (multiplicity) ●	JCD(Hz)	<sup>13</sup> C Chemical Shift (ppm from TMS) (multiplicity) ●	JCD(Hz)	<sup>1</sup> H Chemical Shift of HOD (ppm from TMS) □	Density at 20°C ◆	Melting point (°C) ◆	Boiling point (°C) ◆	Dielectric Constant	Molecular Weight ◆
Acetic Acid-d <sub>4</sub>	11.65 (1) 2.04 (5)	2.2	178.99 (1) 20.0 (7)	20	11.5	1.12	16.7	118	6.1	64.08
Acetone-d <sub>6</sub>	2.05 (5)	2.2	206.68 (1) 29.92 (7)	0.9 19.4	2.8 *	0.87	-94	56.5	20.7	64.12
Acetonitrile-d <sub>3</sub>	1.94 (5)	2.5	118.69 (1) 1.39 (7)	21	2.1 *	0.84	-45	81.6	37.5	44.07
Benzene-d <sub>6</sub>	7.16 (1)		128.39 (3)	24.3	0.4	0.95	5.5	80.1	2.3	84.15
Chloroform-d	7.24 (1)		77.23 (3)	32.0	1.5 *	1.50	-63.5	61-62	4.8	120.38
Cyclohexane-d <sub>12</sub>	1.38 (1)		26.43 (5)	19	0.8	0.89	6.47	80.7	2.0	96.24
Deuterium Oxide	4.80 (DSS) 4.81 (TSP)		NA	NA	4.8	1.11	3.81	101.42	78.5	20.03
N, N-Dimethyl-formamide-d <sub>2</sub>	8.03 (1)		163.15 (3)	29.4	3.5	1.03	-61	153	36.7	80.14
	2.92 (5)	1.9	34.89 (7)	21.0						
	2.75 (5)	1.9	29.76 (7)	21.1						
Dimethyl Sulfoxide-d <sub>6</sub>	2.50 (5)	1.9	39.51 (7)	21.0	3.3 *	1.19	18.45	189	46.7	84.17
1,4-Dioxane-d <sub>8</sub>	3.53 (m)		66.66 (5)	21.9	2.4	1.13	11.8	101.1	2.2	96.16
	5.19 (1)				5.3	0.89	-114.1	78.5	24.5	52.11
Ethanol-d <sub>6</sub>	3.56 (1)		56.96 (5)	22						
	1.11 (m)		17.31 (7)	19						
Methanol-d <sub>4</sub>	4.78 (1)				4.9	0.89	-97.8	64.7	32.7	36.07
	3.31 (5)	1.7	49.15 (7)	21.4						
Methylene Chloride-d <sub>2</sub>	5.32 (3)	1.1	54.00 (5)	27.2	1.5	1.35	-95	39.75	8.9	86.95
	8.74 (1)		150.35 (3)	27.5	5	1.05	-42	115-116	12.4	84.13
Pyridine-d <sub>5</sub>	7.58 (1)		135.91 (3)	24.5						
	7.22 (1)		123.87 (3)	25						
1,1,2,2-Tetrachloroethane-d <sub>2</sub>	6.0		73.78 (3)			1.62	-44	147	8.20	169.86
Tetrahydrofuran-d <sub>8</sub>	3.58 (1)		67.57 (5)	22.2	2.4-2.5	0.99	-108.5	66	7.6	80.16
	1.73 (1)		25.37 (5)	20.2						
Toluene-d <sub>8</sub>			137.86 (1)		0.4	0.94	-95	110.6	2.4	100.19
	7.09 (m)		129.24 (3)	23						
	7.00 (1)		128.33 (3)	24						
	6.98 (5)		125.49 (3)	24						
	2.09 (5)	2.3	20.4 (7)	19						
Trifluoroacetic Acid-d	11.50 (1)		164.2 (4)		11.5	1.41	-15.4	72.4		115.03
			116.6 (4)							
Trifluoroethanol-d <sub>3</sub>	5.02 (1)		126.3 (4)		5	1.41	-43.3	75		103.06
	3.88 (4x3)	2(9)	61.5 (4x5)	22						

S Budavari, M.J. O'Neil, A. Smith, P.E. Heckelman, *The Merck Index, an Encyclopedia of Chemicals, Drugs, and Biologicals - Eleventh Edition*, Merck Co., Inc. Rahway, NJ, 1989.

● The <sup>1</sup>H spectra of the residual protons and <sup>13</sup>C spectra were obtained on a Varian Gemini 200 spectrometer at 295°K. The NMR solvents used to acquire these spectra contain a maximum of 0.05% and 1.0% TMS (v/v) respectively. Since deuterium has a spin of 1, triplets arising from coupling to deuterium have the intensity ratio of 1:1:1. 'm' denotes a broad peak with some fine structures. It should be noted that chemical shifts can be dependent on solvent, concentration and temperature.

□ Approximate values only, may vary with pH, concentration and temperature.

◆ Melting and boiling points are those of the corresponding unlabeled compound (except for D<sub>2</sub>O). These temperature limits can be used as a guide to determine the useful liquid range of the solvents. Information gathered from the Merck Index - Eleventh Edition.

\* HOD Peaks - NMR spectra of "neat" deuterated solvent always exhibit a peak due to H<sub>2</sub>O in addition to the residual solvent peak. When the exchange rate between H<sub>2</sub>O and HDO is slow on the NMR timescale the water peak appears as two peaks, a singlet corresponding to H<sub>2</sub>O and a 1:1:1 triplet corresponding to HDO.

## NMR SOLVENT DATA CHART

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## NMR Solvent Storage and Handling Information

Please note that some packaging sizes of some solvents may require special handling not given below. The bottle or ampoule packaging information should be reviewed for further instructions.

Acetic Acid-d<sub>4</sub> / Acetone-d<sub>6</sub> / Benzene-d<sub>6</sub> / Cyclohexane-d<sub>12</sub> / Deuterium Oxide / N,N-Dimethylformamide-d<sub>7</sub> / Dimethyl Sulfoxide-d<sub>6</sub> / 1,4-Dioxane-d<sub>8</sub> (p-Dioxane) / Ethanol-d<sub>6</sub> / Methanol-d<sub>4</sub> / Methylene Chloride-d<sub>2</sub> / Pyridine-d<sub>5</sub> / 1,1,2,2-Tetrachloroethane-d<sub>2</sub> / Toluene-d<sub>8</sub> / Trifluoroacetic Acid-d / 2,2,2-Trifluoroethanol-d<sub>3</sub>

Store at room temperature away from light and moisture. The above products are stable if stored under recommended conditions.

**Acetonitrile-d<sub>3</sub>**

Store at room temperature away from light and moisture. This product is stable for one year after receipt of order if stored under above conditions (unopened). After one year, the solvent should be re-analyzed for chemical purity before use.

**Chloroform-d / Tetrahydrofuran-d<sub>8</sub>**

Store refrigerated (-5° to 5°C) away from light and moisture. These products are stable for six months after receipt of order if stored under above conditions (unopened). After six months, the solvent should be re-analyzed for chemical purity before use.

**Deuterium exchange of Labile Protons in Deuterated Solvents containing Residual D<sub>2</sub>O**

Some deuterated solvents are prepared by catalytic exchange of protonated solvent with deuterium oxide and carefully purified by distillation. Residual water (H<sub>2</sub>O in equilibrium exchange with D<sub>2</sub>O) is kept to a minimum of 20 - 200 ppm, the higher value corresponds to the amount in the more hygroscopic solvents. The labile deuterons (and protons) of water are available to exchange with labile protons in the chemist's sample and can result in inaccurate integration ratios. The example below shows that just 100 ppm of D<sub>2</sub>O can cause problems when studying dilute solutions of analytes. A significant decrease in the integral of 1 labile proton may be observed in a sample containing 5 mg organic compound, MW~200, dissolved in 1g DMSO-d<sub>6</sub> containing 100 ppm D<sub>2</sub>O. The problem becomes worse as the molecular weight of the analyte increases.

**Solution:**

Water (as H<sub>2</sub>O, HDO or D<sub>2</sub>O) can be minimized by adding molecular sieves to the solvent, agitating the mixture and allowing it to stand for a few hours. The water content may be reduced to about 10-20 ppm in this manner. If exchange still causes a problem, it is recommended to use a less hygroscopic solvent, such as chloroform, methylene chloride or acetonitrile.

**X** – residual solvent; \* – residual water

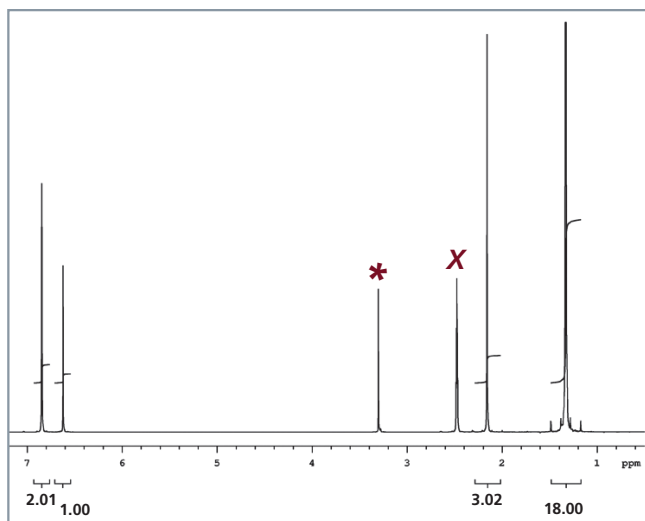


Figure 1- <sup>1</sup>H NMR spectrum of 5.0 mg 2,6-di-tert-butyl-4-methylphenol (MW 220.36g/mole) in dry DMSO-d<sub>6</sub>. Note the proper integral ratios of 18:3:1:2 (t-butyl: methyl: ring-H: -OH). Note the single H<sub>2</sub>O peak at 3.3 ppm.

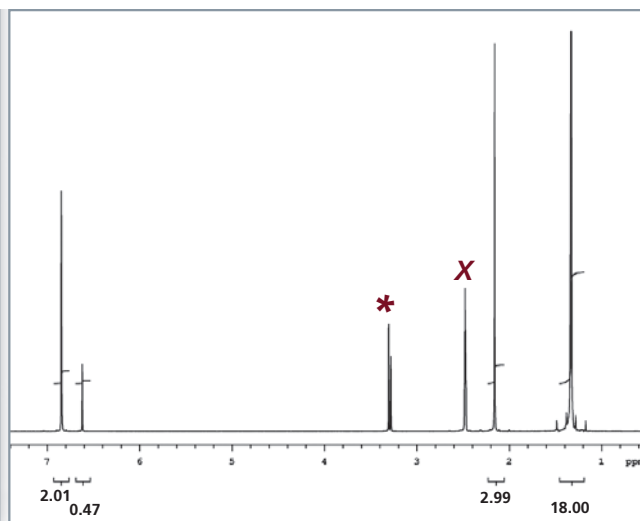


Figure 2- <sup>1</sup>H NMR spectrum of 5.3 mg of 2,6-di-tert-butyl-4-methylphenol in DMSO-d<sub>6</sub> with 100 ppm D<sub>2</sub>O added. Note the reduced ratio of the phenolic proton 18:3:2:0.47 (t-butyl: methyl: ring-H: -OH). Note that the HOH and HOD peaks are separated in the spectrum.



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RESEARCH PRODUCTS

# NMR Solvents

## Chemical Shifts of Selected Compounds in Different Solvents

Compounds	CDCl <sub>3</sub>	(CD <sub>3</sub> ) <sub>2</sub> CO	(CD <sub>3</sub> ) <sub>2</sub> SO	C <sub>6</sub> D <sub>6</sub>	CD <sub>3</sub> CN	CD <sub>3</sub> OD	D <sub>2</sub> O
<b>Solvent residual peak</b>	7.26	2.05	2.50	7.16	1.94	3.31	4.79
<b>H<sub>2</sub>O</b>	1.56	2.84	3.33	0.40	2.13	4.87	
<b>Acetic acid</b>	2.10	1.96	1.91	1.55	1.96	1.99	2.08
<b>Acetone</b>	2.17	2.09	2.09	1.55	2.08	2.15	2.22
<b>Acetonitrile</b>	2.10	2.05	2.07	1.55	1.96	2.03	2.06
<b>Benzene</b>	7.36	7.36	7.37	7.15	7.37	7.33	
<b>tert-butyl alcohol</b>	1.28	1.18	1.11 4.19	1.05 1.55	1.16 2.18	1.40	1.24
<b>tert-butyl methyl ether</b>	1.19 3.22	1.13 3.13	1.11 3.08	1.07 3.04	1.14 3.13	1.15 3.20	1.21 3.22
<b>BTH</b> <i>2,6-Dimethyl-4-tert-butylphenol</i>	6.98 5.01 2.27 1.43	6.96 2.22 1.41	6.87 6.65 2.18 1.36	7.05 4.79 2.24 1.38	6.97 5.20 2.22 1.39	6.92 1.40	
<b>Chloroform</b>	7.26	8.02	8.32	6.15	7.58	7.90	
<b>Cyclohexane</b>	1.43	1.43	1.40	1.40	1.44	1.45	
<b>1,2-Dichloroethane</b>	3.73	3.87	3.90	2.90	3.81	3.78	
<b>Dichloromethane</b>	5.30	5.63	5.76	4.27	5.44	5.49	
<b>Diethyl ether</b>	1.21 3.48	1.11 3.41	1.09 3.38	1.11 3.26	1.12 3.42	1.18 3.49	1.17 3.56
<b>Diglyme</b>	3.65 3.57 3.39	3.56 3.47 3.28	3.51 3.38 3.24	3.46 3.34 3.11	3.53 3.45 3.29	3.61 3.58 3.35	3.67 3.61 3.37
<b>1,2-Dimethoxyethane</b>	3.40 3.55	3.28 3.46	3.24 3.43	3.12 3.33	3.28 3.45	3.35 3.52	3.37 3.60
<b>Dimethylacetamide</b>	2.09 3.02 2.94	1.97 3.00 2.83	1.96 2.94 2.78	1.60 2.57 2.05	1.97 2.96 2.83	2.07 3.31 2.92	2.08 3.06 2.90
<b>Dimethylformamide</b>	8.02 2.96 2.88	7.96 2.94 2.78	7.95 2.89 2.73	7.63 2.36 1.86	7.92 2.89 2.77	7.97 2.99 2.86	7.92 3.01 2.85
<b>Dimethyl sulfoxide</b>	2.62	2.52	2.54	1.68	2.50	2.65	2.71
<b>Dioxane</b>	3.71	3.59	3.57	3.35	3.60	3.66	3.75
<b>Ethanol</b>	1.25 3.72 1.32	1.12 3.57 3.39	1.06 3.44 4.63	0.96 3.34	1.12 3.54 2.47	1.19 3.60	1.17 3.65
<b>Ethyl acetate</b>	2.05 4.12 1.26	1.97 4.05 1.20	1.99 4.03 1.17	1.65 3.89 0.92	1.97 4.06 1.20	2.01 4.09 1.24	2.07 4.14 1.24
<b>Ethyl methyl ketone</b>	2.14 2.46 1.06	2.07 2.45 0.96	2.07 2.43 0.91	1.58 1.81 0.85	2.06 2.43 0.96	2.12 2.50 1.01	2.19 3.18 1.26
<b>Ethylene glycol</b>	3.76	3.28	3.34	3.41	3.51	3.59	3.65
<b>"grease"</b>	0.86 1.26	0.87 1.29		0.92 1.36	0.86 1.27	0.88 1.29	
<b>n-Hexane</b>	0.88 1.26	0.88 1.28	0.86 1.25	0.89 1.24	0.89 1.28	0.90 1.29	
<b>HMPA</b> Hexamethylphosphoramide	2.65	2.59	2.53	2.40	2.57	2.64	2.61
<b>Methanol</b>	3.49 1.09	3.31 3.12	3.16 4.01	3.07	3.28 2.16	3.34	3.34
<b>Nitromethane</b>	4.33	4.43	4.42	2.94	4.31	4.34	4.40
<b>n-Pentane</b>	0.88 1.27	0.88 1.27	0.86 1.27	0.87 1.23	0.89 1.29	0.90 1.29	
<b>2-Propanol</b>	1.22 4.04	1.10 3.90	1.04 3.78	0.95 3.67	1.09 3.87	1.50 3.92	1.17 4.02
<b>Pyridine</b>	8.62 7.29 7.68	8.58 7.35 7.76	8.58 7.39 7.79	8.53 6.66 6.98	8.57 7.33 7.73	8.53 7.44 7.85	8.52 7.45 7.87
<b>Silicone grease</b> Poly(dimethylsiloxane)	0.07	0.13		0.29	0.08	0.10	
<b>Tetrahydrofuran</b>	1.85 3.76	1.79 3.63	1.76 3.60	1.40 3.57	1.80 3.64	1.87 3.71	1.88 3.74
<b>Toluene</b>	2.36 7.17 7.25	2.32 7.1-7.2 7.1-7.2	2.30 7.18 7.25	2.11 7.02 7.13	2.33 7.1-7.3 7.1-7.3	2.32 7.16 7.16	
<b>Triethylamine</b>	1.03 2.53	0.96 2.45	0.93 2.43	0.96 2.40	0.96 2.45	1.05 2.58	0.99 2.57

H. Gottlieb, V. Kotlyar, A. Nudelman, *NMR Chemical Shifts of Common Laboratory Solvents as Trace Impurities*, *J. Org. Chem.*, 62, 1997.