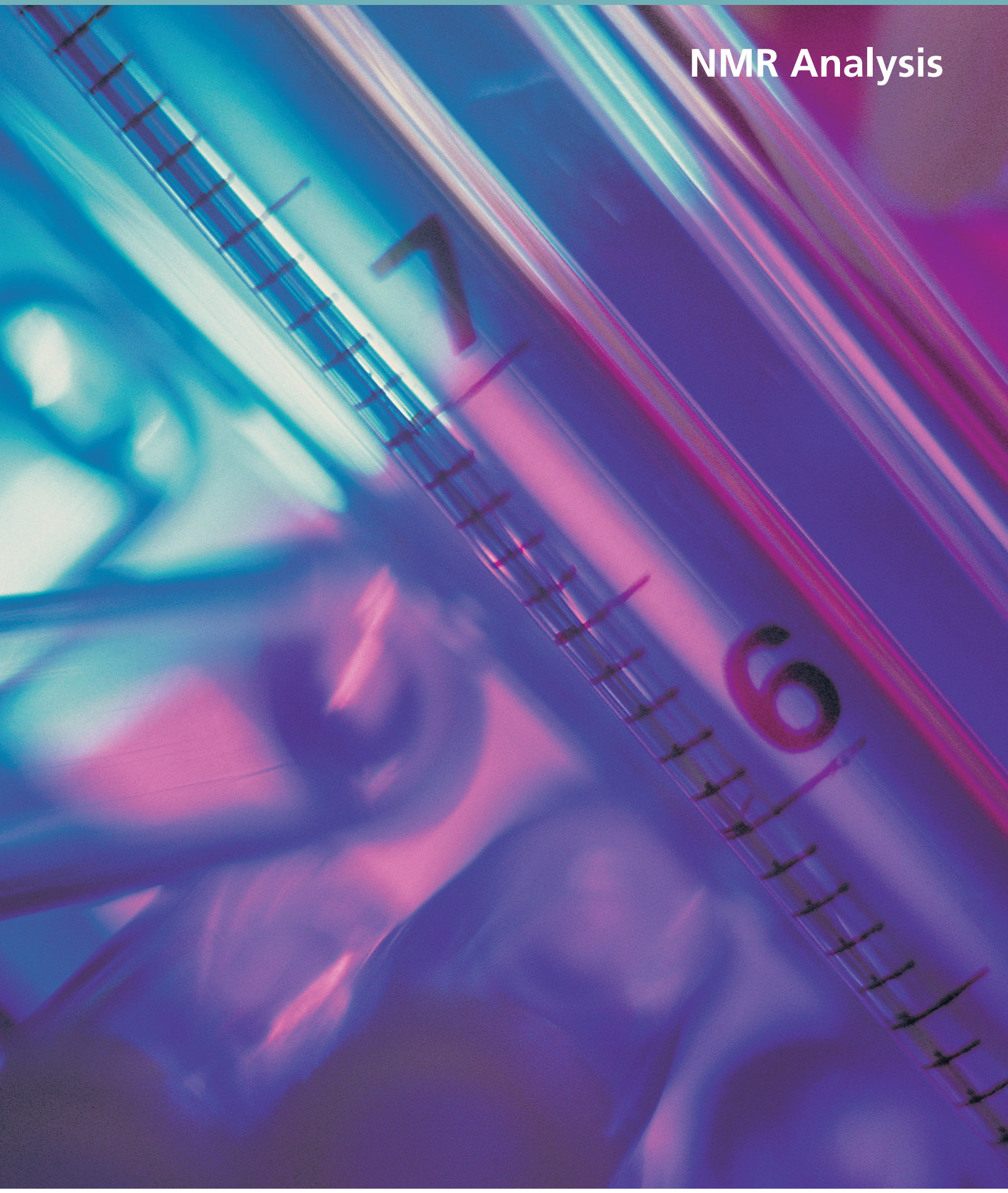
NMR Analysis



About Our Solvents

CIL's NMR solvents are the preferred solvents worldwide for academic, pharmaceutical, industrial and government researchers.

CIL has two dedicated NMR spectrometers for in-process testing, as well as three additional NMR spectrometers in its Quality Control department. Every lot of CIL solvent is routinely tested for both chemical and isotopic purity prior to release to inventory. ^{1}H-NMR data is acquired for each solvent produced, and some solvents are tested for purity by GC/MS for contaminants that would not be observed by ^{1}H-NMR.

CIL's Quality Control Department tests for water content in solvents using the Karl Fischer titration method, and deuterated choloroform is tested for presence of phosgene. All chlorinated solvents are tested for acidity.

CIL's solvents are packaged under an argon or nitrogen atmosphere to ensure the purity is not compromised during packaging. CIL uses amber ampoules and bottles to protect photosensitive solvents from degradation. Every bottle or box of ampoules is clearly marked with a lot number for proper identification.

Acetic acid-d_4 (D, 99.5%)

DLM-12 [1186-52-3] UN# 2789	CD_3COOD	mw 64.08 d 1.12	10 g 25 g 50 g

Acetic acid-d_4 "100%" (D, 99.93%)

DLM-41 [1186-52-3] UN# 2789	CD_3COOD	mw 64.08 d 1.12	10 x 0.75 mL 5 mL

Acetone-d_6 (D, 99.9%)

DLM-9 [666-52-4] UN# 1090	CD_3COCD_3	mw 64.12 d 0.87	10 x 0.5 mL 10 x 0.6 mL 10 x 0.75 mL 5 x 3 mL 1 L 10 x 1 g 3 x (10 x 1 g) 10 g 10 x 10 g 3 x (10 x 10 g) 25 g 100 g

Acetone-d_6 (D, 99.9%)

DLM-9ta [666-52-4] UN# 1090	CD_3COOD_3 *Contains 1% v/v TMS*	mw 64.12 d 0.87	10 x 1 g 3 x (10 x 1 g) 10 g 10 x 10 g 3 x (10 x 10 g) 25 g

Acetone-d_6 (D, 99.9%)

DLM-9tb [666-52-4] UN# 1090	CD_3COCD_3 *Contains 0.05% v/v TMS*	mw 64.12 d 0.87	NEW 10 x 0.5 mL 10 x 1 g 3 x (10 x 1 g) 10 g 10 x 10 g 3 x (10 x 10 g) 25 g

Acetone-d_6 "100%" (D, 99.96%)

DLM-38 [666-52-4] UN# 1090	CD_3COCD_3	mw 64.12 d 0.87	5 x 0.5 mL 10 x 0.5 mL 10 x 0.6 mL 5 x 0.75 mL 10 x 0.75 mL 5 mL

Acetone-d_6 "100%" (D, 99.96%)

DLM-38tc [666-52-4] UN# 1090	CD_3COCD_3 *Contains 0.03% v/v TMS*	mw 64.12 d 0.87	10 x 0.75 mL

Acetonitrile-d_3 (D, 96-97%)

DLM-22 [2206-26-0] UN# 1648	$CD_3C{\equiv}N$	mw 44.07 d 0.84	1 L

Acetonitrile-d_3 (D, 99.8%)

DLM-21 [2206-26-0] UN# 1648	$CD_3C{\equiv}N$	mw 44.07 d 0.84	10 x 0.5 mL 10 x 0.6 mL 10 x 0.75 mL 1 L 10 x 1 g 3 x (10 x 1 g) 5 g 10 g 25 g 50 g

Acetonitrile-d_3 (D, 99.8%)

DLM-21tb [2206-26-0] UN# 1648	$CD_3C{\equiv}N$ *Contains 0.05% v/v TMS*	mw 44.07 d 0.84	10 x 0.6 mL

Acetonitrile-d_3 "100%" (D, 99.96%)

DLM-53 [2206-26-0] UN# 1648	$CD_3C{\equiv}N$	mw 44.07 d 0.84	10 x 0.5 mL 10 x 0.6 mL 5 x 0.75 mL 10 x 0.75 mL 5 mL

Benzene-d_6 (D, 99.5%)

DLM-1 [1076-43-3] UN# 1114	C_6D_6	mw 84.15 d 0.95	10 x 0.5 mL 10 x 0.6 mL 10 x 0.75 mL 10 x 1 g 3 x (10 x 1 g) 5 g 10 g 10 x 10 g 25 g 50 g 100 g 1000 g

Benzene-d_6 (D, 99.5%)

DLM-1tb [1076-43-3] UN# 1114	C_6D_6	mw 84.15 d 0.95	10 x 0.6 mL 10 g

Contains 0.05% v/v TMS

Benzene-d_6 "100%" (D, 99.96%)

DLM-40 [1076-43-3] UN# 1114	C_6D_6	mw 84.15 d 0.95	5 x 0.5 mL 10 x 0.5 mL 5 x 0.75 mL 10 x 0.6 mL 10 x 0.75 mL 5 mL

Benzene-d_6 "100%" (D, 99.96%)

DLM-40tc [1076-43-3] UN# 1114	C_6D_6	mw 84.15 d 0.95	10 x 0.75 mL

Contains 0.03% v/v TMS

Bromobenzene-d_5 (D, 99.5%)

DLM-9595 [4165-57-5] UN# 2514	C_6D_5Br	mw 162.04 d 1.52	5 g 10 g 25 g

Chlorobenzene-d_5 (D, 99%)

DLM-263 [3114-55-4] UN# 1134	C_6D_5Cl	mw 117.59 d 1.16	1 g 5 g

Chloroform-d (D, 99.8%)

DLM-7 [865-49-6] UN# 1888	$CDCl_3$	mw 120.38 d 1.50	10 x 0.6 mL 10 x 0.75 mL 10 x 1 g 3 x (10 x 1 g) 50 g 100 g 10 x 100 g 3 x (10 x 100 g)

No stabilizers are used in this product

Chloroform-d (D, 99.8%)

DLM-7-50S DLM-7-100S [865-49-6] UN# 1888	$CDCl_3$	mw 120.38 d 1.50	50 g 100 g NEW 100 mL

Stabilized with silver foil

Chloroform-d (D, 99.8%)

DLM-7ta [865-49-6] UN# 1888	$CDCl_3$	mw 120.38 d 1.50	10 x 1 g 3 x (10 x 1 g) 50 g 100 g 10 x 100 g 3 x (10 x 100 g)

No stabilizers are used in this product

Chloroform-d (D, 99.8%)

DLM-7ta-100S [865-49-6] UN# 1888	$CDCl_3$	mw 120.38 d 1.50	100 g

Stabilized with silver foil

Chloroform-d "100%" (D, 99.96%)

DLM-7tb [865-49-6] UN# 1888	$CDCl_3$	mw 120.38 d 1.50	10 x 1 g 3 x (10 x 1 g) 50 g 100 g 10 x 100 g 3 x (10 x 100 g)

No stabilizers are used in this product

Chloroform-d (D, 99.8%)

DLM-7tb-50S DLM-7tb-100S [865-49-6] UN# 1888	$CDCl_3$	mw 120.38 d 1.50	50 g 100 g

Stabilized with silver foil

Chloroform-d "100%" (D, 99.96%)

DLM-29 [865-49-6] UN# 1888	$CDCl_3$	mw 120.38 d 1.50	10 x 0.25 mL 10 x 0.5 mL 10 x 0.6 mL 5 x 0.75 mL 10 x 0.75 mL 10 mL 5 x 10 mL 50 g

No stabilizers are used in this product

Chloroform-d "100%" (D, 99.96%)

DLM-29tc [865-49-6] UN# 1888	$CDCl_3$	mw 120.38 d 1.50	10 x 0.75 mL

Contains 0.03% v/v TMS
No stabilizers are used in the product

Cyclohexane-d_{12} (D, 99.5%)

DLM-17 [1735-17-7] UN# 1145	C_6D_{12}	mw 96.23 d 0.89	5 x 1 g 10 x 1 g 3 x (10 x 1 g) 5 g 10 g

Decalin-d_{18} (D, 99%) Decahydronaphthalene

DLM-1386 [28788-42-3]	$C_{10}D_{18}$	mw 156.36 d 1.01	1 g 5 g

cis/trans mixture

trans-Decalin-d_{18} (D, 98%)

DLM-1843 [493-02-7] | $C_{10}D_{18}$ | mw 156.36, d 1.01 | 5 g

Deuterium bromide (D, 99%)

DLM-3021 [13536-59-9] | DBr | mw 81.92, d 1.537 | 10 g (of soln.), 50 g (of soln.)

DBr 48% w/w solution in D_2O
Packaged in clear glass ampoules only

Deuterium chloride (D, 99.5%)

DLM-2 [7698-05-7] | DCl | mw 37.47, d 1.20 | 50 g (of soln.)

DCl 20% w/w solution in D_2O
Packaged in clear glass ampoules only

Deuterium chloride "100%" (D, 99.96%)

DLM-54 [7698-05-7] | DCl | mw 37.47, d 1.20 | 5 g (of soln.), 25 g (of soln.)

DCl 20% w/w solution in D_2O
Packaged in clear glass ampoules only

Deuterium chloride (D, 99.5%)

DLM-3 [7698-05-7] | DCl | mw 37.47, d 1.20 | 50 g (of soln.)

DCl 35% w/w solution in D_2O
Packaged in clear glass ampoules only

Deuterium oxide (D, 70%)

DLM-4-70 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.077 | 1 kg

Deuterium oxide (D, 70%)

DLM-2259-70 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.077 | 1 kg, 1 L

Sterility tested

Deuterium oxide (D, 99%)

DLM-4-99 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 1 kg, 5 kg

Deuterium oxide (D, 99.8%)

DLM-4-99.8 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 1 kg, 10 kg, 20 kg

Deuterium oxide (D, 99.8%)

DLM-2259 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 100 mL, 250 mL, 1 L

Sterility tested

Deuterium oxide (D, 99.9%)

DLM-4 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 10 x 1 mL, 10 g, 25 g, 50 g, 100 g, 5 x 100 g, 10 x 100 g, 1000 g, 1 L (inquire)

Deuterium oxide (D, 99.9%)

DLM-11 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 100 g

Glass distilled, low paramagnetic, low conductivity
Packaged in plastic bottles only

Deuterium oxide "100%" (D, 99.96%)

DLM-6 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 10 x 0.6 mL, 5 x 0.7 mL, 10 x 0.7 mL, 10 x 0.75 mL, 5 x (10 x 0.7 mL), 10 x 1 g, 1000 g

Deuterium oxide "100%" (D, 99.96%)

DLM-6-s [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 10 g

Packaged in serum bottles with Teflon-coated rubber septum tops

Deuterium oxide "100%" (D, 99.96%)

DLM-6DB [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 10 x 0.7 mL, 50 g

Contains 0.01 mg/mL DSS

Deuterium oxide "100%" (D, 99.96%)

DLM-1172 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 10 g

Highest purity, glass distilled, low paramagnetic, low conductivity. Packaged in plastic bottles only.

1-2,Dibromoethane-d_4 (D, 99%)

DLM-195 [22581-63-1] UN# 1605 | $Br(CD_2)_2Br$ | mw 191.87, d 2.20 | 10 g, 25 g

1-2,Dichlorobenzene-d_4 (D, 99%)

DLM-158 [2199-69-1] UN# 1591 | $C_6D_4Cl_2$ | mw 151.03, d 1.34 | 1 g, 5 g, 25 g

1-2,Dichloroethane-d_4 (D, 99%)

DLM-18 [17060-07-0] UN# 1184 | $Cl(CD_2)_2Cl$ | mw 102.98, d 1.30 | 1 g, 5 x 1 g, 5 g

Diethyl ether-d_{10} (D, 99%)

DLM-1592 [2679-89-2] UN# 1155 | $(CD_3CD_2)_2O$ | mw 84.10, d 0.80 | 1 g, 5 x 1 g, 5 g

Packaged in ampoules only

Diglyme-d_{14} (D, 98%)

DLM-47 [38086-00-9] — $(CD_3OCD_2CD_2)_2O$ — mw 148.26, d 1.035 — 1 g, 5 g, 5 x 1 g, 10 g

N,N-Dimethylformamide-d_7 (D, 99.5%) DMF

DLM-25 [4472-41-7] — $DCON(CD_3)_2$ — mw 80.14, d 1.04 — 5 x 1 g, 10 x 1 g, 5 g, 10 g

Packaged in ampoules only

N,N-Dimethylformamide-d_7 (D, 99.5%) DMF

DLM-25tb [4472-41-7] — $DCON(CD_3)_2$ — mw 80.14, d 1.04 — 10 x 0.6 mL

Contains 0.05% v/v TMS
Packaged in ampoules only

Dimethyl sulfoxide-d_6 (D, 99.9%) DMSO

DLM-10 [2206-27-1] — CD_3SOCD_3 — mw 84.17, d 1.18 — 10 x 0.5 mL, 10 x 0.6 mL, 10 x 0.75 mL, 5 x 3 mL, NEW 10 mL, NEW 50 mL, 5 x 1 g, 10 x 1 g, 3 x (10 x 1 g), 5 g, 10 g, 100 g, 10 x 10 g, 3 x (10 x 10 g), 25 g, 50 g, 1000 g

Dimethyl-sulfoxide-d_6 (D, 99.9%) DMSO

DLM-10-s [2206-27-1] — CD_3SOCD_3 — mw 84.17, d 1.18 — NEW 10 mL, 10 g, 25 g

Packaged in serum bottles with Teflon-coated rubber septum tops

Dimethyl-sulfoxide-d_6 (D, 99.9%) DMSO

DLM-10ta [2206-27-1] — CD_3SOCD_3 — mw 84.17, d 1.18 — 10 x 1 g, 3 x (10 x 1) g, 5 g, 10 g, 10 x 10 g, 3 x (10 x 10) g, 25 g, 50 g

Contains 1% v/v TMS

Dimethyl-sulfoxide-d_6 (D, 99.9%) DMSO

DLM-10tb [2206-27-1] — CD_3SOCD_3 — mw 84.17, d 1.18 — NEW 10 x 0.5 mL, 10 x 0.6 mL, 10 x 0.7 mL, 10 x 0.75 mL, 10 x 1 g, 3 x (10 x 1 g), 5 g, 10 g, 10 x 10 g, 3 x (10 x 10 g), 25 g, 50 g, NEW 100 g

Contains 0.05% v/v TMS

Dimethyl-sulfoxide-d_6 "100%" (D, 99.96%) DMSO

DLM-34 [2206-27-1] — CD_3SOCD_3 — mw 84.17, d 1.18 — 10 x 0.25 mL, 5 x 0.5 mL, 10 x 0.5 mL, 10 x 0.6 mL, 5 x 0.75 mL, 10 x 0.75 mL, 5 mL

Dimethyl-sulfoxide-d_6 "100%" (D, 99.96%) DMSO

DLM-34tc [2206-27-1] — CD_3SOCD_3 — mw 84.17, d 1.18 — 10 x 0.75 mL

Contains 0.03% v/v TMS

1,4-Dioxane-d_8 (D, 99%) *p*-Dioxane

DLM-28 [17647-74-4] — $C_4D_8O_2$ — mw 96.15, d 1.13 — 5 x 1 g, 10 x 1 g, 3 x (10 x 1 g), 5 g, 10 g, 25 g

UN# 1165

DSS – ^{1}H-NMR chemical shift standard

DLM-8206 [2039-96-5] — $(CH_3)_3Si(CD_2)_3SO_3Na$ — mw 224.4 — 1 g

UN# 1165

Sodium 2,2-dimethyl-2-silapentane-5-sulfonate (D_6 98%)
Chemical purity 97%

DSS – ^{1}H-NMR chemical shift standard

DLM-32 [2039-96-5] — $(CH_3)_3Si(CH_2)_3SO_3Na$ — mw 218.3 — 1 g, 10 g, 50 g

UN# 1165

Sodium 2,2-dimethyl-2-silapentane-5-sulfonate
Chemical purity 97%

Ethanol-d (D, 99%) Ethyl alcohol

DLM-16 [925-93-9] — CH_3CH_2OD — mw 47.08, d 0.82 — 50 g, 2 x 50 g

UN# 1170

Contains ≤6% D_2O

Ethanol-d_6 (D, 99%) Ethyl alcohol

DLM-31 [1516-08-1] — CD_3CD_2OD — mw 52.11, d 0.89 — 5 x 1 g, 10 x 1 g, 5 g

UN# 1170 3

Anhydrous

Ethanol-d_6 (D, 99%) Ethyl alcohol

DLM-31B [1516-08-1] — CD_3CD_2OD — mw 52.11, d 0.89 — 5 x 1 g, 5 g

UN# 1170 3

Contains ≤6% D_2O

Ethylene glycol-d_6 (D, 98%)

DLM-132 [15054-86-1] — $DOCD_2CD_2OD$ — mw 68.11, d 1.22 — 5 g

Fluorobenzene-d_5 (D, 98%)

DLM-617 [1423-10-5] UN# 2387 — C_6D_5F — mw 101.13, d 1.08 — 1 g

_n_-Heptane-d_{16} (D, 98%)

DLM-423 [33838-52-7] UN# 1206 — $CD_3(CD_2)_5CD_3$ — mw 116.30, d 0.794 — 1 g, 5 g

Hexafluoroacetone trideuterate (D, 99.5%)

DLM-1020 [109640-39-3] — $CF_3COCF_3 \cdot 3\ D_2O$ — mw 226.11, d 1.71 — 10 g

1,1,1,3,3,3-Hexafluoroisopropanol-d_2 (D, 98%)

DLM-143 [38701-74-5] — $(CF_3)_2CDOD$ — mw 170.05, d 1.62 — 1 g, 5 x 1 g, 5 g, 10 g

Hexafluoroisopropyl alcohol, HFIP

_n_-Hexane-d_{14} (D, 98%)

DLM-139 [21666-38-6] UN# 1208 — $CD_3(CD_2)_4CD_3$ — mw 100.26, d 0.767 — 1 g, 5 g

Isopropanol-d_8 (D, 99%) 2-Propyl alcohol

DLM-44 [22739-76-0] UN# 1219 — $(CD_3)_2CDOD$ — mw 68.14, d 0.90 — 5 g, 25 g

Lithium deutoroxide (D, 99.5%)

DLM-2173 [12159-20-5] — LiOD — mw 24.96, d 1.218 — 25 g, 100 g

3N in D_2O solution
Packaged in plastic bottles only

Methanol-d (D, 99%) Methyl alcohol

DLM-15 [1455-13-6] UN# 1230 — CH_3OD — mw 33.05, d 0.81 — 50 g, 2 x 50 g

Methanol-d_4 (D, 99.8%) Methyl alcohol

DLM-24 [811-98-3] UN# 1230 — CD_3OD — mw 36.07, d 0.89 — 10 x 0.5 mL, 10 x 0.6 mL, 10 x 0.75 mL, 1 L, NEW 5 x 1 g, 10 x 1 g, 3 x (10 x 1 g), 5 g, 10 g, 10 x 10 g, 25 g, 50 g, 1000 g

Methanol-d_4 (D, 99.8%) Methyl alcohol

DLM-24-s [811-98-3] UN# 1230 — CD_3OD — mw 36.07, d 0.89 — 10 g, 25 g, 50 g

Packaged in serum bottles with Teflon-coated rubber septum tops

Methanol-d_4 (D, 99.8%) Methyl alcohol

DLM-24tb [811-98-3] UN# 1230 — CD_3OD — mw 36.07, d 0.89 — NEW 10 x 0.5 mL, 10 x 0.6 mL, 10 x 0.75 mL, 10 x 1 g, 10 g, 10 x 10 g, NEW 50 g

Contains 0.05% v/v TMS

Methanol-d_4 "100%" (D, 99.95%) Methyl alcohol

DLM-51 [811-98-3] UN# 1230 — CD_3OD — mw 36.07, d 0.89 — 10 x 0.25 mL, 5 x 0.5 mL, 10 x 0.5 mL, 10 x 0.6 mL, 5 x 0.75 mL, 10 x 0.75 mL

Methylcyclohexane-d_{14} (D, 99.5%)

DLM-288 [10120-28-2] UN# 2296 — $C_6D_{11}CD_3$ — mw 112.27, d 0.88 — 1 g, 5 g

Methylene chloride-d_2 (D, 99.9%) Dichloromethane

DLM-23 [1665-00-5] UN# 1593 — CD_2Cl_2 — mw 86.95, d 1.30 — NEW 10 x 0.5 mL, 10 x 0.75 mL, 5 x 3 mL, 5 x 1 g, 10 x 1 g, 3 x (10 x 1 g), 5 g, 10 g, 25 g, NEW 100 g

Methylene chloride-d_2 (D, 99.9%) Dichloromethane

DLM-23tb [1665-00-5] UN# 1593 — CD_2Cl_2 — mw 86.95, d 1.35 — 10 x 0.6 mL

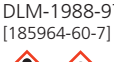
Contains 0.05% v/v TMS

Methylene chloride-d_2 "100%" (D, 99.96%) Dichloromethane

DLM-55 [1665-00-5] UN# 1593 — CD_2Cl_2 — mw 86.95, d 1.35 — 10 x 0.5 mL, 10 x 0.6 mL, 5 x 0.75 mL, 10 x 0.75 mL, 5 mL

_N_-Methyl-2-pyrrolidinone-d_9 (D, 97-99%) NMP

DLM-1988-97 [185964-60-7] — mw 108.19, d 1.13 — Please Inquire



Nitric acid-d (D, 99%)

DLM-3037 [13587-52-5] — DNO_3 — mw 64.02, d 1.026 — 5 g (of soln.), 25 g (of soln.)

65-70% w/w solution in D_2O
Packaged in clear glass ampoules only

Nitrobenzene-d_5 (D, 99%)

DLM-294 [4165-60-0] UN# 1662 — $C_6D_5NO_2$ — mw 128.14, d 1.25 — 5 g, 10 g, 25 g

Nitromethane-d_3 (D, 99%)

DLM-30 [13031-32-8] UN# 1261 — CD_3NO_2 — mw 64.06, d 1.20 — 10 g, 25 g

***n*-Octane-d_{18}** (D, 99%)

DLM-50 [17252-77-6] UN# 1262 — $CD_3(CD_2)_6CD_3$ — mw 132.34, d 0.815 — 1 g, 5 g

***n*-Pentane-d_{12}** (D, 98%)

DLM-1213 [2031-90-5] UN# 1265 — $CD_3(CD_2)_3CD_3$ — mw 84.22, d 0.73 — 1 g, 5 g

Phosphoric acid-d_3 (D, 99%)

DLM-1132 [14335-33-2] — D_3PO_4 — mw 101.01, d 1.74 — 50 g, 100 g

Approximately 85% w/w solution in D_2O

Pyridine-d_5 (D, 99.5%)

DLM-13 [7291-22-7] UN# 1282 — C_5D_5N — mw 84.13, d 1.05 — 10 x 0.5 mL, 5 x 1 g, 10 x 1 g, 3 x (10 x 1 g), 10 g, 25 g, 50 g

Pyridine-d_5 (D, 99.5%)

DLM-13tb [7291-22-7] UN# 1282 — C_5D_5N — mw 84.13, d 1.05 — NEW 10 x 0.5 mL, 10 x 0.6 mL, 5 x 1 g, 10 x 1 g, 3 x (10 x 1 g), 10 g, 25 g, 50 g

Contains 0.05% v/v TMS

Pyridine-d_5 "100%" (D, 99.94%)

DLM-39 [7291-22-7] UN# 1282 — C_5D_5N — mw 84.13, d 1.05 — 5 x 0.5 mL, 10 x 0.5 mL, 5 x 0.75 mL, 10 x 0.75 mL, 5 mL

Sodium deuteroxide (D, 99.5%)

DLM-57 [14014-06-3] UN# 1282 — NaOD — mw 41.00, d 1.46 — 50 g

NaOD 30% w/w solution in D_2O
Packaged in polyethylene bottles

Sodium deuteroxide (D, 99.5%)

DLM-45 [14014-06-3] UN# 1282 — NaOD — mw 41.00, d 1.46 — 50 g, 100 g

NaOD 40% w/w solution in D_2O
Packaged in polyethylene bottles

Sulfuric acid-d_2 (D, 99%)

DLM-33 [13813-19-9] UN# 1282 — D_2SO_4 — mw 100.09, d 1.86 — 50 g

96-98% solution in D_2O
Packaged in glass ampoules only

1,1,2,2-Tetrachloroethane-d_2 (D, 99.6%) TCE

DLM-35 [33685-54-0] UN# 1702 — $Cl_2CDCDCl_2$ — mw 169.86, d 1.62 — 5 g, 10 g, 100 g

Tetrahydrofuran-d_8 (D, 99.5%) THF

DLM-36 [1693-74-9] UN# 2056 — mw 80.16, d 0.99 — NEW 10 x 0.5 mL, 10 x 0.75 mL, 5 x 3 mL, 5 x 1 g, 10 x 1 g, 3 x (10 x 1 g), 5 g, 10 g

Packaged in ampoules only

Tetrahydrofuran-d_8 "100%" (D, 99.95%) THF

DLM-56 [1693-74-9] UN# 2056 — mw 80.16, d 0.99 — 10 x 0.5 mL, 10 x 0.75 mL, 5 mL

Tetramethylsilane TMS

DLM-43 [75-76-3] — $(CH_3)_4Si$ — mw 88.22, d 0.64 — 50 g

NMR grade
Chemical purity 99.9%

TMSP-2,2,3,3-d_4 (D, 98%) Sodium 3-trimethylsilylpropionate

DLM-48 [24493-21-8] — $(CH_3)_3SiCD_2CD_2CO_2Na$ — mw 172.27, d 1.52 — 1 g, 5 x 1 g, 5 g

D_2O reference standard and
^1H-NMR chemical shift standard

Toluene-d_8 (D, 99.5%)

DLM-5 [2037-26-5] UN# 1294 — $C_6D_5CD_3$ — mw 100.19, d 0.94 — 10 x 1 g, 3 x (10 x 1 g), 5 g, 10 g, 25 g, 100 g, 1000 g

Toluene-d_8 "100%" (D, 99.94%)

DLM-42 [2037-26-5] UN# 1294 — $C_6D_5CD_3$ — mw 100.19, d 0.94 — 5 x 0.5 mL, 10 x 0.5 mL, 5 x 0.75 mL, 10 x 0.75 mL, 5 mL

Trifluoroacetic acid-d (D, 99.5%)

DLM-46 [599-00-8] UN# 2699	CF_3COOD	mw 115.03 d 1.50	NEW 10 x 0.5 mL 10 x 0.75 mL 10 x 1 g 10 g 25 g 4 x 25 g

Packaged in ampoules only

2,2,2-Trifluoroethanol-d$_2$ (D, 98%) Trifluoroethyl alcohol

DLM-2318 [77253-67-9]	CF_3CD_2OH	mw 102.05 d 1.37	1 g 5 g

2,2,2-Trifluoroethanol-d$_3$ (D, 99%) Trifluoroethyl alcohol

DLM-27 [77253-67-9]	CF_3CD_2OD	mw 103.06 d 1.42	1 g 5 x 1 g

2,2,2-Trifluoroethanol-d$_3$ "100%" (D, 99.85%) Trifluoroethyl alcohol

DLM-58 [77253-67-9]	CF_3CD_2OD	mw 103.06 d 1.42	1 g 5 g

1,3,5-Trimethyl benzene (D_{12}, 98%) Mesitylene

DLM-3105 [69441-16-3] UN# 2325	$C_3D_3(CD_3)_3$	mw 132.26	5 g

Water, deuterium depleted

DLM-52 [7732-18-5]	H_2O	mw 18.02 d 1.00	25 g 100 g

2-3 ppm deuterium

***o*-Xylene-d$_{10}$** (D, 98%)

DLM-808 [56004-61-6] UN# 1307	$C_6D_4(CD_3)_2$	mw 116.23 d 0.953	5 g

***p*-Xylene-d$_{10}$** (D, 98%)

DLM-313 [41051-88-1] UN# 1307	$C_6D_4(CD_3)_2$	mw 116.23 d 0.948	5 g

^{12}C and ^{12}C/Deuterium-Labeled Solvents (^{13}C Depleted)

Benzene ($^{12}C_6$, 99.95%)

CLM-867 [71-43-2]	$*C_6H_6$	mw 78.05 d 0.874	0.8 mL

^{13}C depleted

Chloroform (^{12}C, 99.95%; D, 99%)

CDLM-844 [865-49-6]	$*CDCl_3$	mw 120.38 d 1.500	Inquire

^{13}C depleted

Glycerol ($^{12}C_3$, 99.95%; D_8, 98%)

CDLM-8660 [56-81-5]	$DO*CD_2*CD(OD)*CD_2OD$	mw 100.11 d 1.250	1g 5g 10g

^{13}C depleted

Methanol (^{12}C, 99.95%) Methyl alcohol

CLM-2472 [67-56-1]	$*CH_3OH$	mw 32.04 d .0791	1 g

^{13}C depleted

Methanol (^{12}C, 99.95%; D_4, 99.5%) Methyl alcohol

CDLM-01 [811-98-3]	$*CD_3OD$	mw 36.07 d 0.888	0.8 mL 5g

^{13}C depleted

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. These standards help to assure proper spectrometer performance. CIL's total quality-assurance protocols and in-house manufacturing capabilities guarantee the highest level of quality the first time, and every time. The NMR reference standards have been evaluated and determined to meet or exceed industry requirements. A representative listing of CIL's most popular NMR reference standards is provided below.

***All reference standards are filled to 2±0.12 inch except for ULM-71 and ULM-69, which are filled to 0.79±0.12 inch, unless noted otherwise.**

Catalog No.	Description	Application	Tube Size
DLM-79	1% 1,2-Dichlorobenzene in acetone-d_6 (D, 99.9%)	^{1}H-Resolution	5 mm x 8"
DLM-74	0.1% Ethylbenzene + 0.01% TMS in chloroform-d "100%" (D, 99.96%)	^{1}H-Sensitivity	5 mm x 8"
DLM-67	1% 3-Heptanone in chloroform-d (D, 99.8%)	^{1}H APT Test	5 mm x 8"
ULM-73	12% TMS in chloroform	^{1}H-Reference/Calibration	5 mm x 8"
DLM-84	5% Ethylbenzene + 2% TMS in chloroform-d (D, 99.8%)	^{1}H-Sensitivity/Reference	5 mm x 8"
DLM-76	1% Chloroform in acetone-d_6 (D, 99.9%)	^{1}H-Line Shape	5 mm x 8"
DLM-90	0.1 mg/mL $GdCl_3 \cdot 6H_2O$ in D_2O (D, 99.96%)	^{1}H-Homogeneity	5 mm x 8"
DLM-72	40% *p*-Dioxane in benzene-d_6 (D, 99.6%)	^{13}C-Sensitivity/Resolution	5 mm x 8"
DLM-66	30% Menthol (by weight) in chloroform-d (D, 99.8%)	^{13}C App Test	5 mm x 8"
DLM-68	90% Formamide in DMSO-d_6 (D, 99.9%)	^{15}N-Sensitivity	5 mm x 8"
DLM-77	0.0485 M Triphenylphosphate in chloroform-d (D, 99.8%)	^{31}P-Sensitivity	5 mm x 8"
DLM-78	0.05% α,α,α,-Trifluorotoluene in benzene-d_6 (D, 99.6%)	^{19}F-Sensitivity	5 mm x 8"
CDLM-100	0.1% Methanol-^{13}C + 0.3 mg/mL $GdCl_3$ in 98.9% D_2O + 01% H_2O	Auto Test Sample	5 mm x 8"
DLM-88	0.1 mg/mL $GdCl_3$ + 0.1% DSS in 20% H_2O in D_2O	Gradient Shimming	5 mm x 8"
CDLM-96	1% $^{13}CH_3I$, 0.2% $Cr(acac)_3$ + 1% $(CH_3O_3)P$ in $CDCl_3$ "100%"	Indirect Detection Test	5 mm x 8"
DNLM-97	0.2% $Cr(acac)_3$ + 2% Benzamide (^{15}N,98%+) in DMSO-d_6 "100%" (D, 99.96%)	Indirect Detection Test	5 mm x 8"
ULM-71	100% Ethylene glycol*	High Temperature Calibrant	5 mm x 8"
ULM-69	100% Methanol*	Low Temperature Calibrant	5 mm x 8"
ULM-92	10% TMS in methanol	Low Temperature Measurement	5 mm x 8"
CDNLM-5003	0.1 M Urea-^{15}N + 0.1 M MeOH-^{13}C in DMSO-d_6 100%	Indirect Detection Experiments	5 mm x 8"
DLM-5022	2% 2-Ethyl-1-indanone in chloroform-d	2D Calibration	5 mm x 8"
CDNLM-7011	0.1% Methanol-^{13}C - 0.1% acetonitrile-^{15}N + 0.3 mg/mL in 98.8% D_2O + 1% H_2O	Auto Test Sample	5 mm x 8"
DLM-7049	5% Ethyl *trans*-crotonate + 1% TMS in $CDCl_3$ in a 7" sealed NMR tube/fill height 50 mm	General Test Sample	5 mm x 7"
ULM-7047	98% *N*-Propyl benzoate + 2% TMS in a 7" sealed NMR tube/fill height 50 mm	General Test Sample	5 mm x 7"
DLM-5001	10% Ethylbenzene in chloroform-d (540 pp tube)	^{13}C Sensitivity	5 mm x 8"

CIL's Commitment

CIL is committed to assisting you with your research by providing **customized solvent mixtures**, **buffers** and **NMR standards**. We welcome your requests for **custom formulations** or **other reference standards**, as well as **alternative fill heights** of existing **reference standards**. To submit a custom request, please contact your local CIL representative.

Phone: 1.800.322.1174 (North America)
+1.978.749.8000 (International)
Fax: 978.749.2768
Email: cilsales@isotope.com

Requests may be submitted on our website at isotope.com/request.

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Special Purpose High-Throughput NMR Sample Tubes

Part No.	Package Size	MHz Rating	O.D. (mm)	I.D. (mm)	Length (inch)	Concentricity (mm)	Camber (mm)
502-7	50	100	4.97 ± 0.050	4.20 ± 0.050	7	0.020	0.070
502-8	50	100	4.97 ± 0.050	4.20 ± 0.050	8	0.020	0.070

Standard Series for Routine NMR

Part No.	Package Size	MHz Rating	O.D. (mm)	I.D. (mm)	Length (inch)	Concentricity (µm)	Camber (µm)
507-HP-7	5	400	4.97 ± 0.013	4.20 ± 0.025	7	0.0070	0.019
507-HP-8	5	400	4.97 ± 0.013	4.20 ± 0.025	8	0.0070	0.019
508-UP-7	5	500	4.97 ± 0.013	4.20 ± 0.025	7	0.0050	0.013
508-UP-8	5	500	4.97 ± 0.013	4.20 ± 0.025	8	0.0050	0.013
XR-55-7	25	300	4.97 ± 0.025	4.20 ± 0.025	7	0.010	0.038
XR-55-8	25	300	4.97 ± 0.025	4.20 ± 0.025	8	0.010	0.038

Select Series for High-Resolution NMR

Part No.	Package Size	MHz Rating	O.D. (mm)	I.D. (mm)	Length (inch)	Concentricity (µm)	Camber (µm)
S-5-200-7	5	200	4.97 ± 0.030	4.20 ± 0.030	7	0.0090	0.0350
S-5-200-8	5	200	4.97 ± 0.030	4.20 ± 0.030	8	0.0090	0.0350
S-5-300-7	5	300	4.97 ± 0.025	4.20 ± 0.025	7	0.0070	0.0250
S-5-300-8	5	300	4.97 ± 0.025	4.20 ± 0.025	8	0.0070	0.0250
S-5-400-7	5	400	4.97 ± 0.013	4.20 ± 0.025	7	0.0070	0.0190
S-5-400-8	5	400	4.97 ± 0.013	4.20 ± 0.025	8	0.0070	0.0190
S-5-500-7	5	500	4.97 ± 0.013	4.20 ± 0.025	7	0.0050	0.0130
S-5-500-8	5	500	4.97 ± 0.013	4.20 ± 0.025	8	0.0050	0.0130
S-5-600-7	5	600	4.97 ± 0.006	4.20 ± 0.012	7	0.0040	0.0060

CIL provides a wide selection of NMR tubes. Download a complete guide to help you find the right one for your next research project.
isotope.com/nmrtubes

Wilmad-LabGlass NMR Sample Tubes

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Wilmad LabGlass

www.wilmad-labglass.com

Pyrex® Glass Precision Tubes

5 mm O.D. Precision Tubes

Part No.	MHz Rating	O.D. (mm)	I.D. (mm)	Length (inch)	Wall Thickness (mm)	Concentricity (µm)	Camber (µm)
535-PP-7	600	4.9635±0.0065	4.2065±0.0065	7	0.38	13	6
528-PP-7	500	4.9635±0.0065	4.2065±0.0065	7	0.38	25	13
528-PP-8	500	4.9635±0.0065	4.2065±0.0065	8	0.38	25	13
527-PP-7	400	4.9635±0.0065	4.2065±0.0065	7	0.38	25	25
527-PP-8	400	4.9635±0.0065	4.2065±0.0065	8	0.38	25	25
507-PP-7	300	4.9635±0.0065	4.2065±0.0065	7	0.38	51	25
505-PS-7	100	4.9635±0.0065	4.2065±0.0065	7	0.38	76	51

10 mm O.D. Precision Tubes

Part No.	MHz Rating	O.D. (mm)	I.D. (mm)	Length (inch)	Wall Thickness (mm)	Concentricity (µm)	Camber (µm)
513-7PP-7	500	9.9935±0.0065	9.07±0.013	7	0.46	38	13
513-1PP-7	200	9.9935±0.0065	9.07±0.013	7	0.46	254	51

NMR Quartz Precision Tubes

Part No.	MHz Rating	O.D. (mm)	I.D. (mm)	Length (inch)	Wall Thickness (mm)	Concentricity (µm)	Camber (µm)
535-PP-7QTZ	600	4.9635±0.0065	4.2065±0.0065	7	0.38	13	6
528-PP-7QTZ	500	4.9635±0.0065	4.2065±0.0065	7	0.38	25	13

Coaxial Insert for Samples with Limited Volume

Part No.	MHz Rating	Fits Outer Tube	Stem Height (mm)	Stem O.D. (mm)	Sample Capacity (µL)
WGS-5BL	600	Any Precision Tube with 5 mm O.D., 7" length and 0.38 mm wall thickness	50	2.0195±0.0125	530

Gas-tight NMR Tubes for Air-Sensitive Samples

Part No.	MHz Rating	O.D. (mm)	I.D. (mm)	Tube Length (inch)	Wall Thickness (mm)
528-LPV-7	500	4.9635±0.0065	4.2065±0.0065	7	0.38
507-LPV-7	300	4.9635±0.0065	4.2065±0.0065	7	0.38

N51A Glass Economy Tubes

5 mm O.D. Economy Tubes

Part No.	MHz Rating	O.D. (mm)	Wall Thickness (mm)	Length (inch)	Concentricity (µm)	Camber (µm)
WG-1235-7	>400	4.93395±0.03175	0.43	7	13	6
WG-1228-7	400	4.93395±0.03175	0.43	7	25	13
WG-1228-8	400	4.93395±0.03175	0.43	8	25	13
WG-1226-7	300	4.93395±0.03175	0.43	7	51	13
WG-1226-8	300	4.93395±0.03175	0.43	8	51	13
WG-5MM-ECONOMY-7	100	4.93395±0.03175	0.43	7	76	76
WG-5MM-ECONOMY-8	100	4.93395±0.03175	0.43	8	76	76

Bulk Pack 5 mm Economy Tubes (100 tubes, no cap)

Part No.	MHz Rating	O.D.(mm)	Wall Thickness (mm)	Length (inch)
WG-1000-7	100	4.93395±0.03175	0.43	7

The tube length for the above LPV tubes does not include the valve and the top glass adapter.

Use and Handling of NMR Solvents

CIL has implemented extensive quality-control protocols for the evaluation of chemical and isotopic purities of its 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 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 CIL's 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 dessicator prior to use.
- Precondition an NMR tube by rinsing it with D_2O. Remove residual D_2O by rinsing first with methanol-d_4 or acetone-d_6 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_2O

To avoid loss of enrichment due to exchange with ambient moisture, "100%" D_2O 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_2O being removed should be injected into the serum bottle prior to withdrawing D_2O.

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 a refrigerator; freezing is not recommended. It is recommended that chloroform, diethyl ether, diglyme, tetrahydrofuran and TMS be stored in a refrigerator.

NMR Solvent Technical Tips

- Solvent users often 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. 1960. *J Phys Chem, 64,* 188).
- Dimethyl sulfoxide (DMSO) has a melting point of 18°C, freezing close to room temperature. Upon delivery, DMSO will sometimes 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 serum bottles to extend the product shelf life, maintain high purity and ensure product quality. Serum bottles should be tested after six months.
- It is recommend that chloroform, diethyl ether, diglyme, tetrahydrofuran and TMS be stored in a refrigerator.
- In order to avoid isotopic contamination, some products, especially deuterated compounds, should be handled under an inert atmosphere, such as dry nitrogen or argon.
- You may see a split water peak in your solvent because the Karl Fischer technique measures the total of H_2O + D_2O. In all cases where both H_2O and D_2O are present, there will also be HOD present due to the chemical exchange equilibrium. It is not possible to guarantee there will be no HOD present in the solvents under these circumstances. However, CIL takes great care to minimize the amount of D_2O present in the solvents. Thus, a neglible amount of HOD may remain but will not be observable in the NMR spectrum of most solvents. Occasionally, a separate peak from HOD, ~0.02 ppm upfield of the H_2O peak, may be observed in the DMSO-d_6 or acetronitrile-d_3 (for example), due to the slower equilibrium that exists between H_2O and D_2O and these solvents.
- CIL also specializes in ^{13}C-depleted and deuterium-depleted compounds. Please contact us if you do not see the ^{13}C-depleted/deuterium-depleted compound of interest.
- CIL welcomes your requests for custom formulations of reference standards not listed in this section.
- CIL's NMR solvent data chart is available as a laminated reference document. Please contact your customer account coordinator to request a copy.

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. For international orders, 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 ^{1}H NMR, GC, Karl Fischer 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 between -5°C to +5°C to maximize shelf life. Moisture and oxygen will be introduced to the solvent following initial use due to 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:

- 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 two 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), then the deuterated chloroform is acidic.

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

- Place 3-5 grams of 5Å molecular sieves into a 50 g or 100 g 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 Requiring Ultra-Dry and Acid-Free Deuterated Chloroform

For applications involving highly acid-sensitive or moisture-sensitive compounds, deuterated chloroform can be further purified 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 (~7 mm 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 as dry and free of trace amounts of acid as possible 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.

NMR Solvent Data Chart

More Solvents, More Sizes, More Solutions

	^{1}H Chemical Shift (ppm from TMS) (multiplicity) ❊	JHD (Hz)	^{13}C Chemical Shift (ppm from TMS) (multiplicity) ❊	JCD (Hz)	^{1}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_4	**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_6	**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_3	**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_6	**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_{12}	**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_7	**8.03 (1) 2.92 (5) 2.75 (5)**	**1.9 1.9**	**163.15 (3) 34.89 (7) 29.76 (7)**	**29.4 21.0 21.1**	**3.5**	**1.03**	**-61**	**153**	**36.7**	**80.14**
Dimethyl sulfoxide-d_6	**2.50 (5)**	**1.9**	**39.51 (7)**	**21.0**	**3.3***	**1.19**	**18.55**	**189**	**46.7**	**84.17**
1,4-Dioxane-d_8	**3.53 (m)**		**66.66 (5)**	**21.9**	**2.4**	**1.13**	**11.8**	**101.1**	**2.2**	**96.16**
Ethanol-d_6	**5.19 (1) 3.56 (1) 1.11 (m)**		**56.96 (5) 17.31 (7)**	**22 19**	**5.3**	**0.89**	**-114.1**	**78.5**	**24.5**	**52.11**
Methanol-d_4	**4.87 (1) 3.31 (5)**	**1.7**	**49.15 (7)**	**21.4**	**4.9**	**0.89**	**-97.8**	**64.7**	**32.7**	**36.07**
Methylene chloride-d_2	**5.32 (3)**	**1.1**	**54.00 (5)**	**27.2**	**1.5**	**1.35**	**-95**	**39.75**	**8.9**	**86.95**
Pyridine-d_5	**8.74 (1) 7.58 (1) 7.22 (1)**		**150.35 (3) 135.91 (3) 123.87 (3)**	**27.5 24.5 25**	**5**	**1.05**	**-41.6**	**115.2-115.3**	**12.4**	**84.13**
1,1,2,2-Tetrachloroethane-d_2	**6.0**		**73.78 (3)**			**1.62**	**-44**	**146.5**	**8.20**	**169.86**
Tetrahydrofuran-d_8	**3.58 (1) 1.73 (1)**		**67.57 (5) 25.37 (5)**	**22.2 20.2**	**2.4-2.5**	**0.99**	**-108.5**	**66**	**7.6**	**80.16**
Toluene-d_8	**7.09 (m) 7.00 (1) 6.98 (5) 2.09 (5)**	**2.3**	**137.86 (1) 129.24 (3) 128.33 (3) 125.49 (3) 20.4 (7)**	**23 24 24 19**	**0.4**	**0.94**	**-95**	**110.6**	**2.4**	**100.19**
Trifluoroacetic acid-d	**11.50 (1)**		**164.2 (4) 116.6 (4)**		**11.5**	**1.49**	**-15.4**	**72.4**		**115.03**
Trifluoroethanol-d_3	**5.02 (1) 3.88 (4x3)**	**2(9)**	**126.3 (4) 61.5 (4x5)**	**22**	**5**	**1.41**	**-43.5**	**74.05**		**103.06**

O'Neil, M.J.; Heckelman, P.E.; Koch, C.B.; Roman, K.J. **2006**. *The Merck Index,* an Encyclopedia of Chemicals, Drugs, and Biologicals – Fourteenth Edition, Merck Co., Inc. Whitehouse Station, NJ.

❊ The ^{1}H spectra of the residual protons and ^{13}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_2O). These temperature limits can be used as a guide to determine the useful liquid range of the solvents. Information gathered from the Merck Index – Fourteenth Edition.

* HOD Peaks – NMR spectra of "neat" deuterated solvent always exhibit a peak due to H_20 in addition to the residual solvent peak. When the exchange rate between H_20 and HOD is slow on the NMR timescale the water peak appears as two peaks, a singlet corresponding to H_20 and a 1:1:1 triplet corresponding to HOD.

NMR Solvent Storage and Handling Information

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

Acetic Acid-d_4 / Acetone-d_6 / Benzene-d_6 / Cyclohexane-d_{12} / Deuterium Oxide / *N,N*-Dimethylformamide-d_7 / Dimethyl Sulfoxide-d_6 / 1,4-Dioxane-d_8 (*p*-Dioxane) / Ethanol-d_6 / Methanol-d_4 / Methylene Chloride-d_2 / Pyridine-d_5 / 1,1,2,2-Tetrachloroethane-d_2 / Toluene-d_8 / Trifluoroacetic Acid-d / 2,2,2-Trifluoroethanol-d_3

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

Acetonitrile-d_3

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

Chloroform-d / Tetrahydrofuran-d_8

Store refrigerated between -5° to 5°C away from light and moisture. These products are stable for six months after receipt of order if stored under these 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_2O

Some deuterated solvents are prepared by catalytic exchange of protonated solvent with deuterium oxide and are carefully purified by distillation. Residual water (H_2O in equilibrium exchange with D_2O) 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 figures below show that just 100 ppm of D_2O 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 1 g DMSO-d_6 containing 100 ppm D_2O. The problem becomes worse as the molecular weight of the analyte increases.

Solution

Water (as H_2O, HOD or D_2O) 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*

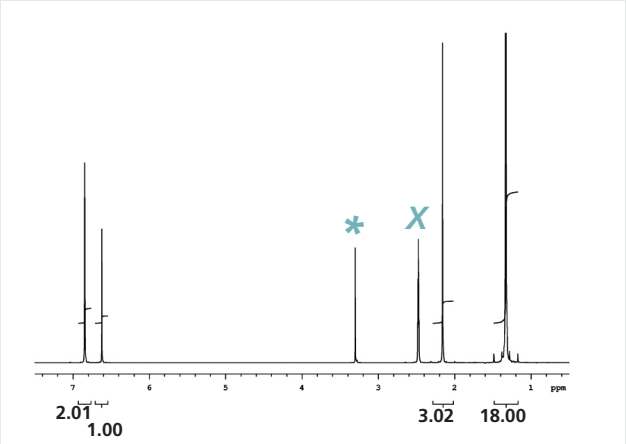

Figure 1. ^{1}H-NMR spectrum of 5.0 mg 2,6-di-*tert*-butyl-4-methylphenol (MW 220.36g / mole) in dry DMSO-d_6. *Note the proper integral ratios of 18:3:1:2 (t-butyl: methyl: ring-H: -OH). Note the single H_2O peak at 3.3 ppm.*

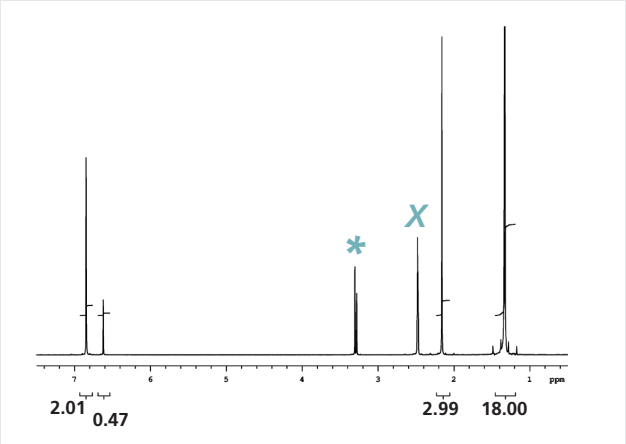

Figure 2. ^{1}H-NMR spectrum of 5.3 mg of 2,6-di-*tert*-butyl-4-methylphenol in DMSO-d_6 with 100 ppm D_2O added. *Note the reduced ratio of the phenolic proton 18:3:2:0.47 (t-butyl: methyl: ring-H: -OH). Note that the HOH and HOD peaks are separated in the spectrum.*

NMR Solvents Chemical Shifts of Selected Compounds in Different Solvents

Compounds	$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
Solvent residual peak	7.26	2.05	2.50	7.16	1.94	3.31	4.79
H_2O	1.56	2.84	3.33	0.40	2.13	4.87	
Acetic acid	2.10	1.96	1.91	1.55	1.96	1.99	2.08
Acetone	2.17	2.09	2.09	1.55	2.08	2.15	2.22
Acetonitrile	2.10	2.05	2.07	1.55	1.96	2.03	2.06
Benzene	7.36	7.36	7.37	7.15	7.37	7.33	
tert-butyl alcohol	1.28	1.18	1.11 4.19	1.05 1.55	1.16 2.18	1.40	1.24
tert-butyl methyl ether	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
BTH – *2,6-Dimethyl-4-tert-butylphenol*	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 2.21 1.40	
Chloroform	7.26	8.02	8.32	6.15	7.58	7.90	
Cyclohexane	1.43	1.43	1.40	1.40	1.44	1.45	
1,2-Dichloroethane	3.73	3.87	3.90	2.90	3.81	3.78	
Dicholoromethane	5.30	5.63	5.76	4.27	5.44	5.49	
Diethyl ether	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
Diglyme	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
1,2-Dimethoxyethane	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
Dimethylacetamide	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
Dimethylformamide	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
Dimethyl sulfoxide	2.62	2.52	2.54	1.68	2.50	2.65	2.71
Dioxane	3.71	3.59	3.57	3.35	3.60	3.66	3.75
Ethanol	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
Ethyl acetate	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
Ethyl methyl ketone	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
Ethylene glycol	3.76	3.28	3.34	3.41	3.51	3.59	3.65
"grease"	0.86 1.26	0.87 1.29		0.92 1.36	0.86 1.27	0.88 1.29	
n-Hexane	0.88 1.26	0.88 1.28	0.86 1.25	0.89 1.24	0.89 1.28	0.90 1.29	
HMPA – Hexamethylphosphoramide	2.65	2.59	2.53	2.40	2.57	2.64	2.61
Methanol	3.49 1.09	3.31 3.12	3.16 4.01	3.07	3.28 2.16	3.34	3.34
Nitromethane	4.33	4.43	4.42	2.94	4.31	4.34	4.40
n-Pentane	0.88 1.27	0.88 1.27	0.86 1.27	0.87 1.23	0.89 1.29	0.90 1.29	
2-Propanol	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
Pyridine	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
Silicone grease – Poly(dimethylsiloxane)	0.07	0.13		0.29	0.08	0.10	
Tetrahydrofuran	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
Toluene	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	
Triethylamine	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

Gottlieb, H.; Kotlyar, V.; Nvdelman, A. **1997**. NMR Chemical Shifts of Common Laboratory Solvents as Trace Impurities. *J Org Chem, 62,* 75-12-7515.