

Everything for NMR Spectroscopy by Carl ROTH



NMR Spectroscopy

NMR spectroscopy has become one of the most important instruments in the field of structure determination of a wide variety of compounds. For example, NMR spectroscopy cannot only be used to determine molecular structures but also to get informations about the identity and purity of substances, molecular conformations and intermolecular interactions.

Generally speaking, the method serves to investigate the electronic environment of individual atoms and thus provides insight into the interactions between neighbouring atoms.

However, certain factors such as the solubility of the sample, the water content and viscosity of the solvent as well as the position of the solvent signals in the spectrum have to be taken into account, when selecting a suitable solvent.

To provide laboratories with support in carrying out such analyses, Carl ROTH offers a range of **deuterated solvents, acids and bases** as well as additional **consumables for NMR spectroscopy**.

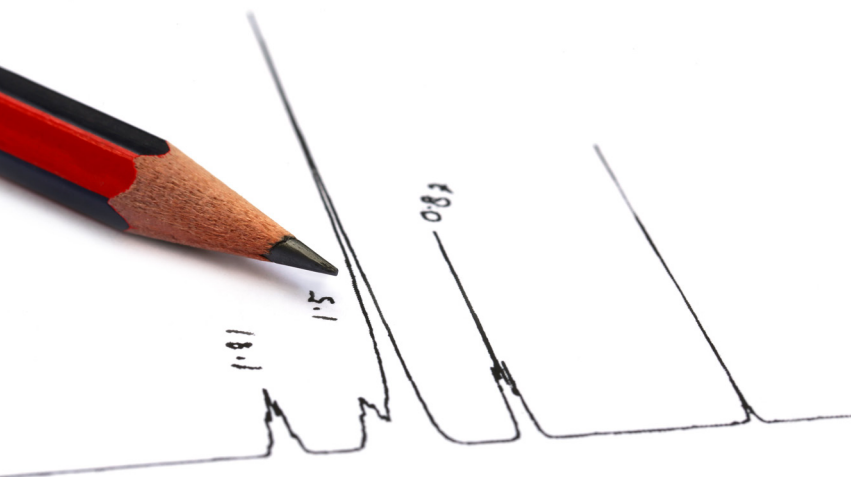


Advantages:

- High degree of deuteration
- Defined water content
- Extremely cost effective

Application examples:

- Routine tasks such as structure determination and identity verification in research and development laboratories
- Elucidation of reaction mechanisms and metabolisms
- For GC-MS or LC-MS as internal standards



Deuterated Solvents



Product name	Purity	Pack.	Art. No.	Pack Qty.
Acetone D6	100 Atom%D	glass ampoule	1K3E.1	7.5 ml
		glass ampoule	AE51.3	7.5 ml
		glass	AE51.1	10 ml
	99,8 Atom%D	septum bottle	AE51.4	10 ml
		glass	AE51.5	25 ml
		glass	AE51.2	50 ml
99,5 Atom%D	glass	7909.1	10 ml	
			7909.2	50 ml
Acetonitrile D3	100 Atom%D	glass ampoule	1K3H.1	7.5 ml
		glass ampoule	7911.2	7.5 ml
		glass	7911.1	10 ml
	99,8 Atom%D	glass	7911.3	25 ml
		glass	AE52.1	10 ml
		septum bottle	AE52.3	10 ml
99,5 Atom%D	glass	AE52.2	25 ml	
	glass ampoule	7912.3	7.5 ml	
	99,8 Atom%D	glass	7912.1	10 ml
glass		7912.2	25 ml	
99,5 Atom%D		glass	AE53.1	10 ml
	septum bottle	AE53.3	10 ml	
	glass	AE53.4	25 ml	
			AE53.2	50 ml
			AE53.5	100 ml
Bromobenzene D5	99,5 Atom%D	glass	HN93.1	10 ml
Chlorobenzene D5	99 Atom%D	glass	9905.1	5 ml
Cyclohexane D12	99,5 Atom%D	glass	5200.1	5 ml
Deuterium oxide	100 Atom%D	glass ampoule	HN81.3	7.5 ml
		glass	HN81.1	10 ml
		septum bottle	HN81.4	10 ml
		glass	HN81.2	50 ml
		glass ampoule	6672.6	7.5 ml
	99,9 Atom%D	glass	6672.1	10 ml
		septum bottle	6672.5	10 ml
		glass	6672.2	25 ml
		glass	6672.3	100 ml
		glass	6672.4	500 ml
			6672.7	1 l
1,2-Dichlorobenzene D4	99 Atom%D	glass	HN82.2	1 ml
			HN82.1	5 ml
Dichloromethane D2	99,8 Atom%D	glass ampoule	7913.2	7.5 ml
		glass	7913.1	10 ml
		glass	AE55.3	5 ml
	99,5 Atom%D	glass ampoule	AE55.5	7.5 ml
		glass	AE55.1	10 ml
		glass	AE55.2	25 ml
			AE55.4	50 ml
Diethyl ether D10	99 Atom%D	glass ampoule	9907.1	1 ml
<i>N,N</i> -Dimethylformamide D7	99,5 Atom%D	glass ampoule	CP92.2	1 ml
		glass	CP92.1	5 ml
Dimethyl sulphoxide D6	100 Atom%D	glass ampoule	1K3K.1	7.5 ml
		glass ampoule	7915.3	7.5 ml
		glass	7915.1	10 ml
	99,9 Atom%D	septum bottle	7915.2	10 ml
		glass ampoule	AE56.3	7.5 ml
		glass	AE56.1	10 ml
	99,8 Atom%D	septum bottle	AE56.4	10 ml
		glass	AE56.6	25 ml
		glass	AE56.2	50 ml
		glass	AE56.5	100 ml

Product name	Purity	Pack.	Art. No.	Pack Qty.
Dimethyl sulphoxide D6 with TMS (0.03 vol.%)	99,9 Atom%D	glass ampoule	7916.1	7.5 ml
		glass ampoule	AE60.3	7.5 ml
	99,8 Atom%D	glass	AE60.1	10 ml
		glass	AE60.2	50 ml
Ethanol D1	99,5 Atom%D	glass	HN84.1	50 ml
Ethanol D6	99 Atom%D	glass	CP93.2	1 ml
			CP93.1	5 ml
Methanol D1	99,5 Atom%D	glass	HN86.1	25 ml
			HN86.2	100 ml
Methanol D3	99,5 Atom%D	glass ampoule	9910.1	1 ml
		glass	9910.2	5 ml
Methanol D4	100 Atom%D	glass ampoule	7918.2	7.5 ml
		glass	7918.1	10 ml
		glass ampoule	AE57.3	7.5 ml
	99,8 Atom%D	glass	AE57.1	10 ml
		septum bottle	AE57.4	10 ml
		glass	AE57.5	25 ml
			AE57.2	50 ml
Methanol D4 with TMS (0.03 vol.%)	99,8 Atom%D	glass ampoule	7919.3	7.5 ml
		glass	7919.1	10 ml
			7919.2	25 ml
Methylcyclohexane D14	99,5 Atom%D	glass	9913.1	5 ml
Nitrobenzene D5	99,5 Atom%D	glass	9914.1	5 ml
			9914.2	10 ml
Nitromethane D3	99 Atom%D	glass	HN91.2	5 ml
			HN91.1	10 ml
2-Propanol D1	98 Atom%D	glass	9917.1	25 ml
2-Propanol D8	99,5 Atom%D	glass	9919.1	5 ml
Pyridine D5	99,8 Atom%D	glass ampoule	7922.2	7.5 ml
		glass	7922.1	10 ml
	99,5 Atom%D	glass ampoule	CP94.3	7.5 ml
		glass	CP94.1	10 ml
		septum bottle	CP94.2	10 ml
Styrene D8	99 Atom%D, stabilised with 4- <i>tert</i> -butylcatechol	glass ampoule	9921.1	1 g
1,1,2,2-Tetrachloroethane D2	99,5 Atom%D	glass ampoule	CP96.2	7.5 ml
		glass	CP96.1	10 ml
		glass ampoule	AE58.3	5 ml
Tetrahydrofuran D8	99,5 Atom%D	glass ampoule	AE58.5	7.5 ml
		glass	AE58.1	10 ml
		septum bottle	AE58.2	10 ml
		glass	AE58.4	25 ml
		glass	AE58.2	25 ml
Toluene D8	99,8 Atom%D	glass ampoule	7924.2	7.5 ml
		glass	7924.1	10 ml
	99,5 Atom%D	glass ampoule	CP95.2	7.5 ml
		glass	CP95.1	10 ml
Trichloromethane/Chloroform D1	100 Atom%D	glass ampoule	CP91.1	7.5 ml
		glass ampoule	7903.1	7.5 ml
	99,8 Atom%D, stabilised with Ag	glass	AE54.4	25 ml
		septum bottle	AE54.1	100 ml
		glass	AE54.2	500 ml
Trichloromethane/Chloroform D1 with TMS (0.03 vol.%)	99,8 Atom%D, stabilised with Ag	glass ampoule	7905.1	7.5 ml
		glass	AE59.1	100 ml

Safety-relevant data and further information in the current catalogue and at www.carlroth.com

Deuterated Acids and Bases

Product name	Purity	Pack.	Art. No.	Pack Qty.
Acetic acid D1	99 Atom%D	glass	9902.1	50 ml
Acetic acid D4	99,5 Atom%D	glass	HN83.1	10 ml
Ammonia-D3 solution 25 % in D ₂ O	99 Atom%D	glass	9903.1	10 ml
Deuterium chloride 38 % solution in D ₂ O	99,5 Atom%D	glass	HN80.1	10 ml
Deuterium chloride 20 % solution in D ₂ O	99,5 Atom%D	glass	1K3L.1	25 ml
Formic acid D 95 % solution in D ₂ O	98 Atom%D	glass	1L35.1	5 ml
Formic acid D2 95 % solution in D ₂ O	98 Atom%D	glass	HN92.1	5 ml
ortho-Phosphoric acid D3, 85 % solution in D ₂ O	99 Atom%D	glass	9915.1	10 ml
		glass	9915.2	25 ml
Pyridine D5	99,8 Atom%D	glass ampoule	7922.2	7.5 ml
		glass	7922.1	10 ml
	99,5 Atom%D	glass ampoule	CP94.3	7.5 ml
		glass septum bottle	CP94.1	10 ml
			CP94.2	10 ml
Sodium deuterium oxide 40 % solution in D ₂ O	99,5 Atom%D	glass	1K3N.1	10 g
Sodium deuterium oxide 30 % solution in D ₂ O	99,5 Atom%D	glass	HN90.1	10 ml
Sulphuric acid D2 98 % solution in D ₂ O	99,5 Atom%D	glass	HN87.1	10 ml
			HN87.2	50 ml
Trifluoroacetic acid D	99,5 Atom%D	glass ampoule	CP97.1	10 ml

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Carl ROTH also offers you a selection of isotope-labeled amino acids (SILAC).



Deuterated Special Compounds

Product name	Purity	Pack.	Art. No.	Pack Qty.
Acetyl chloride D3	99 Atom%D	glass	1L34.1	5 ml
Biphenyl D10	99 Atom%D	glass	1L36.1	1 g
1,4-Dichlorobenzene D4	98 Atom%D	glass	1L37.1	1 g
Dimethyl carbonate D6	99,5 Atom%D	glass	1L38.1	1 ml
1,1,1,3,3,3-Hexafluoro-2-propanol D2 (HFIP-D2)	99 Atom%D	glass ampoule	9909.1	1 ml
Iodomethane D3	99,5 Atom%D, stabilised with Cu	glass	HN88.2	5 g
			HN88.1	25 g
Phenylboronic acid D5	98 Atom%D	glass	1L3A.1	1 g
Sodium borodeuteride	98 Atom%D	glass	HN89.1	1 g
Sodium formate D	99,5 Atom%D	glass	1L39.1	10 g

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Reagents for NMR Calibration

Tetramethylsilane

≥99,9 %, for NMR spectroscopy

For the calibration of NMR spectra; calibration substance.

C₄H₁₂Si · M 88,22 g/mol

Storage temperature: +4 °C

UN no. 2749 · ADR 3 I · WGK 2

Danger H224-H411



Art. No.	Pack Qty.	Pack.
CP18.1	25 ml	glass
CP18.2	100 ml	glass

3-(Trimethylsilyl)propionic-2,2,3,3 acid sodium salt D4 (TSP-D4)

99 Atom%D

For nuclear magnetic resonance spectroscopy.

(CH₃)₃SiCD₂CD₂CO₂Na · M 172,27 g/mol

WGK 1

Warning H315-H319-H335

Art. No.	Pack Qty.	Pack.
9922.1	1 g	plastic

Accessories for NMR Spectroscopy



NMR tube ROTILABO®

ROTH SELECTION. Material: borosilicate glass 3.3.

Technical specifications:

Art. No.	HX58.1	ATP0.1
Version	NMR tubes ROTILABO®	NMR tube ROTILABO® brown
Length	178 ±0,5 mm	
Ø ext.	4,95 ±0,05 mm	4,97 +0,02/-0,05 mm
Ø Internal	4,15 ±0,05 mm	
Straightness	±0,07 mm	
Wall thickness	0,38 mm	
MHz	100-300	
Delivery	without sealing caps, please order separately.	incl. sealing cap made of EVA.

Version	Art. No.	Pack Qty.
NMR tubes ROTILABO®	HX58.1	50 unit(s)



Accessories for NMR tubes

Designation	Art. No.	Pack Qty.
Brush for NMR tubes	KNL1.1	1 unit(s)
Sealing caps for NMR tubes, material: EVA	HX59.1	1,000 unit(s)

A 121 °C

Sample stands for NMR tubes

ROTH SELECTION. Material: PP.

With two handles on the side for easy transportation. Stability is provided by hemispherical holes in the lower level.

- Suitable for NMR tubes Ø 5 mm

No. of slots	L x W x H (mm)	Art. No.	Pack Qty.
72	210 x 110 x 220	YA94.1	1 unit(s)



NMR tubes

DWK Life Sciences.

Tubes do not contain any paramagnetic substances. Excellent straightness, uniform wall thickness, good diameter regularity. With retrace code.

Technical specifications:

Art. No.	EP54.1	KNK9.1	KNL0.1	EP55.1
Version	Economic	Economic 5.1	Professional	Scientific
Length	178 mm			
Ø ext.	4,95 ±0,05 mm	4,94 ± 0,04 mm	4,97 ± 0,025 mm	4,97 ±0,013 mm
Ø Internal	4,20 ±0,05 mm	4,20 ± 0,04 mm	4,20 ± 0,025 mm	4,20 ±0,025 mm
Straightness	±0,07 mm		±0,03 mm	0,013 mm
MHz	300	100	400	500

Delivery incl. sealing caps.

NMR tubes Economic

Material: borosilicate glass 3.3.

For single use in fully automated sample changers or for high throughput.

Version	Art. No.	Pack Qty.
Economic	EP54.1	250 unit(s)

NMR tubes Scientific

Material: borosilicate glass 3.3.

For multiple use. Tubes can be cleaned and sterilised. Optimum substance utilisation in highest resolution range.

Version	Art. No.	Pack Qty.
Scientific	EP55.1	5 unit(s)

NMR tubes Economic 5.1

Material: borosilicate glass 5.1.

For economical use with high throughput in the low-frequency range.

Version	Art. No.	Pack Qty.
Economic 5.1	KNK9.1	100 unit(s)

NMR tubes Professional

Material: borosilicate glass 3.3.

For use in industry and research in the medium and high-resolution range.

Version	Art. No.	Pack Qty.
Professional	KNL0.1	250 unit(s)

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