

¹³C CHEMICAL SHIFTS OF USEFUL NMR SOLVENTS

The following table gives the expected carbon-13 chemical shifts, relative to tetramethylsilane, for various useful NMR solvents. In some solvents, slight changes can occur with change of concentration.^{2,3}

References

1. Bruno, T. J., and Svoronos, P. D. N., *CRC Handbook of Basic Tables for Chemical Analysis*, CRC Press, Boca Raton, FL, 1989.
2. Silverstein, R. M., Bassler, G. C., and Morrill, T. C., *Spectrometric Identification of Organic Compounds*, John Wiley & Sons, New York, 1981.
3. Rahman, A. U., *Nuclear Magnetic Resonance. Basic Principles*, Springer-Verlag, New York, 1986.
4. Pretsch, E., Clerc, T., Seibl, J., and Simon, W., *Spectral Data for Structure Determination of Organic Compounds, Second Edition*, Springer-Verlag, Heidelberg, 1989.

Solvent	Formula	Chemical shift (ppm)
Acetic acid- <i>d</i> ₄	CD ₃ COOD	20.0 (CD ₃) 205.8 (C=O)
Acetone	(CH ₃) ₂ C=O	30.7 (CH ₃) 206.7 (C=O)
Acetone- <i>d</i> ₆	(CD ₃) ₂ C=O	29.2 (CD ₃) 204.1 (C=O)
Acetonitrile- <i>d</i> ₃	CD ₃ C≡N	1.3 (CD ₃) 117.1 (C≡N)
Benzene	C ₆ H ₆	128.5
Benzene- <i>d</i> ₆	C ₆ D ₆	128.4
Carbon disulfide	CS ₂	192.3
Carbon tetrachloride	CCl ₄	96.0
Chloroform	CHCl ₃	77.2
Chloroform- <i>d</i> ₃	CDCl ₃	77.05
Cyclohexane- <i>d</i> ₁₂	C ₆ D ₁₂	27.5
Dichloromethane- <i>d</i> ₂	CD ₂ Cl ₂	53.6
Dimethylformamide- <i>d</i> ₇	(CD ₃) ₂ NCDO	31 (CD ₃) 36 (CD ₃) 162.4 (C=O)
Dimethylsulfoxide- <i>d</i> ₆	(CD ₃) ₂ S=O	39.6
Dioxane- <i>d</i> ₈	C ₄ D ₃ O ₂	67.4
Formic acid- <i>d</i> ₂	DCOOD	165.5
Methanol- <i>d</i> ₄	CD ₃ OD	49.3
Nitromethane- <i>d</i> ₃	CD ₃ NO ₂	57.3
Pyridine	C ₅ H ₅ N	123.6 (C ₃) 135.7 (C ₄) 149.8 (C ₂)
Pyridine- <i>d</i> ₅	C ₅ D ₅ N	123.9 (C ₃) 135.9 (C ₄) 150.2 (C ₂)
1,1,2,2-Tetrachloroethane- <i>d</i> ₂	CDCl ₂ CDCl ₂	75.5
Tetrahydrofuran- <i>d</i> ₈	C ₄ D ₈ O	25.8 (C ₂) 67.9 (C ₁)
Trichlorofluoromethane	CFCl ₃	117.6