

CHEMICAL SHIFT REFERENCE AND STANDARD SAMPLE

Nuclide	Reference (0ppm)	Secondary standard material	Shift* /ppm
¹ H	Tetramethylsilane(TMS)	benzene	6.771 (0.005)
		CHCl ₃	7.392 (0.005)
		H ₂ O	4.877 (0.005)
		adamantane	1.91 (0.01)
		Si(SiMe ₃) ₄	0.247 (0.011)
		Silicone rubber (spinning \cong 2.5kHz)	0.119(0.003)
² H	D ₂ O	D ₂ O	0
⁷ Li	1.0M LiCl aqueous-solution	LiCl	-1.19(0.03)
		LiBr	-2.04(0.03)
¹¹ B	(C ₂ H ₅) ₂ O•BF ₃	H ₃ BO ₃ saturated-solution	19.49(0.02) *3
		BPO ₄	-3.60(0.03)
		NaBH ₄	-42.06(0.02)
¹³ C	Tetramethylsilane(TMS)	Benzene	128.475(0.005)
		CHCl ₃	77.966(0.005)
		adamantane	38.520(0.005)
			29.472(0.004)
		Glycine	176.46(0.02)
			43.67(0.01)
		Hexamethylbenzene	132.07(0.04)
			17.17(0.02)
	Silicone rubber (spinning \cong 3.0kHz)	1.412(0.004)	
	Si(SiMe ₃) ₄	3.517(0.005)	
¹⁵ N	nitromethane	HCONH ₂	-266.712(0.004)
		¹⁵ NH ₄ Cl	-341.168(0.011)
		NH ₄ Cl(10 at.% ¹⁵ N)	-341.168(0.011)
²³ Na	1.0M NaCl aqueous-solution	NaCl	7.21(0.03)
		NaBr	5.04(0.02)
		NaI	-3.25(0.06)
		NaBH ₄	-8.16(0.02)
²⁷ Al	1.0M Al(NO ₃) ₃ aqueous solution	1.0M AlCl ₃ aqueous solution	-0.10(0.01)
		AlK(SO ₄) ₂ •12H ₂ O	-0.21(0.02)
		AlNH ₄ (SO ₄) ₂ •12H ₂ O	-0.54(0.02)


Nuclide	Reference (0ppm)	Secondary standard material	Shift* /ppm
²⁹ Si	Tetramethylsilane(TMS)	Hexamethylsiloxane	6.679(0.004)
		3-(trimethylsilyl) propionic acid-d1 sodium salt.	1.445*1(0.012)
		3-(trimethylsilyl) propionic acid sodium salt	1.459*1(0.012)
		3-(trimethylsilyl)propane-1-sulphonic acid sodium salt	1.534*1(0.012)
		(4.4-dimatyl-4-silapentanesulphonic acid sodium salt)	-
		Si(SiMe ₃) ₄	9.843(0.006)
			-135.402(0.007)
		Hexamethyl trisiloxane Silicone rubber(spinning ≅ 2.0kHz)	-9.66(0.05) -22.333(0.008)
³¹ P	85% H ₃ PO ₄ aqueous-solution	(NH ₄)H ₂ PO ₄ (NH ₄)H ₂ PO ₄	1.33(0.02) 1.00(0.03)
³⁵ Cl	KCl (solid)	76. 0M NaCl aqueous-solution NaCl KCl	-3.90(0.02) ST*3 -49.73(0.03) 0
³⁹ K	1.0M KCl aqueous-solution	KCl KBr KI	47.8(0.1) ST*3 55.1(0.1) ST*3 59.3(0.1) ST*3
⁵¹ V	VO ₃ Cl	0.16M NaVO ₃ aqueous-solution	-574.28(0.05) ST*3
⁵⁹ Co	K ₃ Co(CN) ₆ saturated aqueous solution	K ₃ Co(CN) ₆ saturated aqueous-solution	0 ST*3
⁶³ Cu	CuCl (solid)	CuCl	0
⁶⁵ Cu	CuCl (solid)	CuCl	0
⁷⁷ Se	Se(CH ₃) ₂	(NH ₄) ₂ SeO ₄	1040.20(0.01)
		Na ₂ SeO ₄	1059.18(0.02)
		K ₂ SeO ₄	1052.79(0.03)
⁷⁹ Br	KBr(solid)	76. 0M KBr aqueous-solution NaBr KBr	-42.7(0.1) ST*3 -52.89(0.08) 0
⁸⁷ Rb	1.0M RbCl aqueous-solution	RbCl	123.43(0.06)
¹¹⁹ Sn	Tetramethyltin	SnO ₂	-602.77(0.02)
		Na ₂ SnO ₃ ·3H ₂ O	-563.78(0.03)
		K ₂ SnO ₃ ·3H ₂ O	-569.11(0.02)

Nuclide	Reference (0ppm)	Secondary standard material	Shift* /ppm
¹²⁵ Te	(CH ₃) ₂ Te	76. 0M K ₂ TeO ₃ aqueous-solution Te(OH) ₆	1736.6(0.1) ST*3 692.20(0,10) 685.53(0.13)
¹²⁷ I	KI(solid)	76. 0M KI aqueous solution NaI KI PbI	-168.7(0.6) ST*3 33.53(0.23) 0 76.91(0.12)
¹³³ Cs	1.0M CsCl aqueous solution	CsCl	218.52(0.14)
¹⁹⁵ Pt	Tetramethylsilane (TMS) (1H x 0.214)	0.9M H ₂ PtCl ₆ 10% HCl aqueous solution (294K) (NH ₄) ₂ PtCl ₆ (300K) K ₂ PtCl ₆ (300K)	4521.1(0.2) ST*3 4737.3*1(0.2) 4704.8*1(0.2)

*1: Express the peak position measured using the instrument with 400MHz for ¹H resonance frequency. Shift correction accompanied with second order quadrupolar interaction has not been carried out. The numerical value in parentheses expresses the error range.

*3: The value attached ST obtains without MAS. Even if ST is not indicated as to the value in liquid, the value is obtained under MAS.

*4: Although it is a spectrum with fine structure, it expresses the position of a central peak.

 The above "Chemical shift reference and standard sample" is referred from "Solid NMR of material seen in chart" issued 1993.