4.5 CHARTS FOR MULTINUCLEAR NMR MEASUREMENTS

This section contains useful data for multinuclear NMR measurements.

4.5.1 Relationships Nuclear Species

● Relative sensitivity

The ^{13}C sensitivity reference is taken as 1.00.

Table 4.4 Nuclei table

Nucleus	Natural abundance, percent	Nuclear spin	Relative sensitivity	Reference	Solvent	J_{XH} range
^{1}H	99.985	1/2	5.7×10^{3}	$(CH_3)_4Si$	$CDCl_3$	—
^{2}H	1.5×10^{-2}	1	8.2×10^{-3}	$(CH_3)_4Si$	$CDCl_3$	—
^{3}H		1/2	6.9×10^{3}	$(CH_3)_4Si$	$CDCl_3$	—
^{6}Li	7.42	1	3.58	LiCl	D_2O	—
^{7}Li	92.58	3/2	1.5×10^{3}	LiCl	D_2O	—
^{9}Be	100	–3/2	7.9×10^{1}	$Be(NO_3)_2$	D_2O	—
^{10}B	19.58	3	2.2×10^{1}	$NaBH_4$	D_2O	—
^{11}B	80.42	3/2	7.54×10^{2}	$NaBH_4$	D_2O	30 to 182
^{13}C	1.108	1/2	1.00	$(CH_3)_4Si$	$CDCl_3$	—
^{14}N	99.63	1	5.7	CH_3NO_2	$CDCl_3$	60 to 140
^{15}N	0.37	–1/2	2.2×10^{-2}	CH_3NO_2	$CDCl_3$	60 to 140
^{17}O	3.7×10^{-2}	–5/2	6.1×10^{-2}	D_2O	D_2O	80 to 85
^{19}F	100	1/2	4.7×10^{3}	CF_3COOH	$CDCl_3$	—
^{23}Na	100	3/2	5.25×10^{2}	NaBr	D_2O	—
^{25}Mg	10.13	–5/2	1.5	$MgCl_2$	D_2O	—
^{27}Al	100	5/2	1.7×10^{2}	$Al(NO_3)_3$	D_2O	110 to 185
^{29}Si	4.70	–1/2	2.1	$(CH_3)_4Si$	$CDCl_3$	150 to 420
^{31}P	100	1/2	3.77×10^{2}	H_3PO_4	D_2O	40 to 1,100
^{33}S	0.76	3/2	9.7×10^{-2}	$(NH_4)_2SO_4$	D_2O	—
^{35}Cl	75.53	3/2	2.2	KCl	D_2O	41 (HCl)
^{37}Cl	24.47	3/2	3.8	KCl	D_2O	41 (HCl)
^{39}K	93.10	3/2	2.7	KBr	D_2O	—
^{41}K	6.86	3/2	3.3×10^{-2}	KBr	D_2O	—
^{43}Ca	0.145	–7/2	5.27×10^{-2}	$CaCl_2$	D_2O	—
^{45}Sc	100	7/2	1.7×10^{3}	$ScCl_3$	D_2O	—
^{47}Ti	7.28	–5/2	0.87	$TiCl_4$	—	—
^{49}Ti	5.51	–7/2	1.18	$TiCl_4$	—	—
^{50}V	0.24	6	0.75	$VOCl_3$	C_6D_6	—
^{51}V	99.76	7/2	2.15×10^{3}	$VOCl_3$	C_6D_6	—
^{53}Cr	9.55	–3/2	0.49	$CrO_4(NH_4)_2$	D_2O	—

Nucleus	Natural abundance, percent	Nuclear spin	Relative sensitivity	Reference	Solvent	J_{XH} range
^{55}Mn	100	5/2	9.94×10^{2}	$KMnO_4$	D_2O	—
^{57}Fe	2.19	1/2	4.2×10^{-3}	$Fe(CO)_5$	C_6D_6	—
^{59}Co	100	7/2	1.57×10^{3}	$K_3Co(CN)_6$	D_2O	—
^{61}Ni	1.19	–3/2	0.24	$Ni(CO)_4$	C_6D_6	—
^{63}Cu	69.09	3/2	3.65×10^{2}	CuCN	D_2O	—
^{65}Cu	30.91	3/2	2.01×10^{2}	CuCN	D_2O	—
^{67}Zn	4.11	5/2	0.665	$Zn(NO_3)_2$	D_2O	—
^{69}Ga	60.4	3/2	2.73×10^{2}	$Ga(NO_3)_3$	D_2O	—
^{71}Ga	39.6	3/2	3.19×10^{2}	$Ga(NO_3)_3$	D_2O	—
^{73}Ge	7.76	–9/2	0.617	$Ge(CH_3)_4$	C_6D_6	97.6 (GeH_4)
^{75}As	100	3/2	1.43×10^{2}	$NaAsF_6$	—	90 to 555
^{77}Se	7.58	1/2	3.0	$Se(CH_3)_2$	C_6D_6	40 to 65
^{79}Br	50.54	3/2	2.26×10^{2}	NaBr	D_2O	62 (Hbr)
^{81}Br	49.46	3/2	2.77×10^{2}	NaBr	D_2O	62 (Hbr)
^{85}Rb	72.15	5/2	4.3×10^{1}	RbCl	D_2O	—
^{87}Rb	27.85	3/2	2.77×10^{2}	RbCl	D_2O	—
^{87}Sr	7.02	–9/2	1.1	$SrCl_2$	D_2O	—
^{89}Y	100	–1/2	0.668	$Y(NO_3)_3$	D_2O	—
^{91}Zr	11.23	–5/2	6.04	$(C_2H_5)_2ZrCl_2$	—	—
^{93}Nb	100	9/2	2.74×10^{3}	$NbCl_6$	CD_3CN	—
^{95}Mo	15.72	5/2	2.9	Na_2MoO_4	D_2O	—
^{97}Mo	9.46	–5/2	1.8	Na_2MoO_4	D_2O	—
^{99}Ru	12.72	–3/2	0.83	RuO_4	—	—
^{101}Ru	17.07	–5/2	1.56	RuO_4	—	—
^{103}Rh	100	–1/2	0.18	$RhCl_6^{3-}$	D_2O	15 to 30
^{105}Pb	22.23	–5/2	1.41	K_2PdCl_6	D_2O	—
^{107}Ag	51.82	–1/2	0.2	$AgNO_3$	D_2O	—
^{109}Ag	48.18	–1/2	0.28	$AgNO_3$	D_2O	—
^{111}Cd	12.75	–1/2	6.9	$Cd(CH_3COO)_2$	D_2O	—
^{113}Cd	12.26	–1/2	7.6	$Cd(CH_3COO)_2$	D_2O	—
^{113}In	4.28	9/2	8.4×10^{1}	$In(NO_3)_3$	D_2O	—
^{115}In	95.72	9/2	1.9×10^{3}	$In(NO_3)_3$	D_2O	—
^{117}Sn	7.61	–1/2	2.0×10^{1}	$(CH_3)_4Sn$	$CDCl_3$	110 to 2 450
^{119}Sn	8.58	–1/2	2.5×10^{1}	$(CH_3)_4Sn$	$CDCl_3$	110 to 2 450
^{121}Sb	57.25	5/2	5.2×10^{1}	$KSbCl_6$	CD_3CN	—
^{123}Sb	42.75	7/2	1.11×10^{1}	$KSbCl_6$	CD_3CN	—
^{123}Te	6.99	–1/2	1.3×10^{1}	$(CH_3)_2Te$	C_6D_6	—
^{125}Te	0.87	–1/2	0.89	$(CH_3)_2Te$	C_6D_6	—
^{127}I	100	5/2	5.30×10^{2}	KI	D_2O	—
^{129}Xe	26.44	1/2	3.2×10^{1}	Xe(Gas)	—	—

Nucleus	Natural abundance, percent	Nuclear spin	Relative sensitivity	Reference	Solvent	J_{XH} range
^{133}Cs	100	7/2	2.69×10^{2}	$CsNO_3$	D_2O	—
^{135}Ba	6.59	3/2	1.8	$BaCl_2$	D_2O	—
^{137}Ba	11.32	3/2	4.4	$BaCl_2$	D_2O	—
^{139}La	99.911	7/2	3.4×10^{2}	$LaCl_3$	D_2O	—
^{141}Pr	100	5/2	1.7×10^{5}	—	—	—
^{143}Nd	12.18	–7/2	2.33×10^{2}	—	—	—
^{145}Nd	8.30	–7/2	3.7×10^{1}	—	—	—
^{147}Sm	15.0	–7/2	1.25×10^{2}	—	—	—
^{149}Sm	13.8	–7/2	5.9×10^{1}	—	—	—
^{151}Eu	47.8	5/2	4.8×10^{4}	—	—	—
^{153}Eu	52.2	5/2	4.5×10^{3}	—	—	—
^{155}Gd	14.80	–3/2	2.3×10^{1}	—	—	—
^{157}Gd	15.65	–3/2	5.2×10^{1}	—	—	—
^{159}Tb	100	3/2	3.3×10^{4}	—	—	—
^{161}Dy	18.9	5/2	4.5×10^{1}	—	—	—
^{163}Dy	24.9	5/2	1.6×10^{1}	—	—	—
^{165}Ho	100	7/2	1.0×10^{5}	—	—	—
^{167}Er	22.95	–7/2	6.6×10^{1}	—	—	—
^{169}Tm	100	–1/2	3.2	—	—	—
^{171}Yb	14.31	1/2	5.46×10^{-3}	—	—	—
^{173}Yb	16.13	–5/2	1.33×10^{-3}	—	—	—
^{175}Lu	97.41	7/2	3.12×10^{-2}	—	—	—
^{177}Hf	18.5	7/2	6.38×10^{-4}	—	—	—
^{179}Hf	13.75	–9/2	2.16×10^{-4}	—	—	—
^{181}Ta	99.988	7/2	2.0×10^{2}	$KTaCl_6$	—	—
^{183}W	14.40	1/2	6×10^{-2}	Na_2WO_4	D_2O	30 to 80
^{185}Re	37.07	5/2	2.8×10^{2}	$KReO_4$	D_2O	—
^{187}Re	62.93	5/2	4.9×10^{2}	$KReO_4$	D_2O	—
^{187}Os	1.64	1/2	1.1×10^{-3}	OsO_4	—	—
^{189}Os	16.1	3/2	2.1	OsO_4	—	—
^{191}Ir	37.3	3/2	2.0×10^{-2}	—	—	—
^{193}Ir	62.7	3/2	5×10^{-2}	—	—	—
^{195}Pt	33.8	1/2	1.9×10^{1}	Na_2PtCl_4	D_2O	700 to 1 300
^{197}Au	100	3/2	6×10^{-2}	—	—	—
^{199}Hg	16.84	1/2	5.4	$(CH_3)_2Hg$	C_6D_6	—
^{201}Hg	13.22	–3/2	1.1	$(CH_3)_2Hg$	C_6D_6	—
^{203}Tl	29.50	1/2	2.89×10^{2}	$Tl(NO_3)_3$	D_2O	—
^{207}Pb	22.6	1/2	1.18×10^{1}	$Pb(NO_3)_2$	D_2O	—
^{209}Bi	100	9/2	7.77×10^{2}	$Bi(NO_3)_3$	—	—

4.5.2 Multinuclear NMR Chemical Shifts

The main reason to perform multinuclear NMR is to determine chemical shift values. Unfortunately, it may take a considerable amount of time to find a signal of a new nucleus or an unknown sample due to the wide chemical shift ranges in multinuclear NMR. However, if the chemical shift range for the nucleus or sample under study can be estimated, or if the chemical shift value of a similar compound is known, the time required to find the signal can be substantially reduced.
To assist in this estimation, reported experimental data for chemical shift ranges of the following nuclei are shown below: ^{11}B, ^{13}C, ^{14}N/^{15}N, ^{17}O, ^{19}F, ^{27}Al, ^{29}Si, ^{31}P, ^{33}S, ^{59}Co, ^{67}Zn, ^{75}As, ^{77}Se, ^{103}Rh, ^{109}Ag, ^{113}Cd, ^{119}Sn, ^{195}Pt, ^{199}Hg, ^{207}Pb. The vertical lines in the figure show the positions of the signals. If the signal has two or more lines, these are also indicated. When you measure a new nucleus or an unknown sample, it is recommended that you use these chemical shift figures.

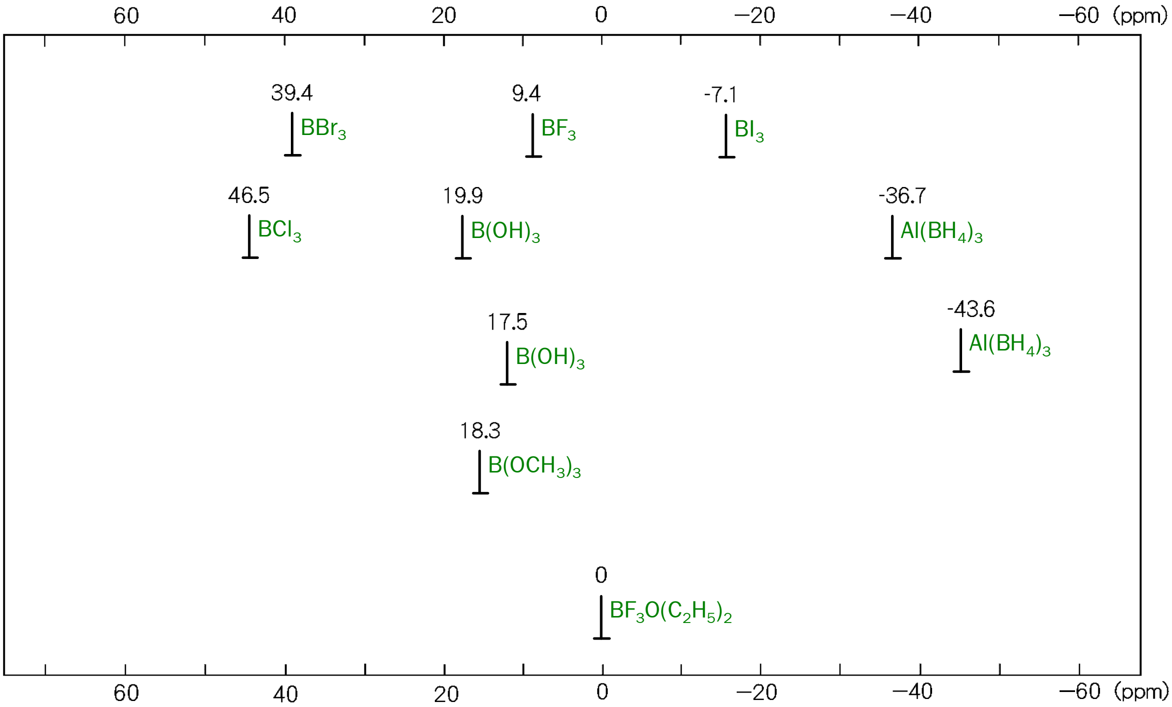

Figure 4.3 ^{11}B chemical shifts

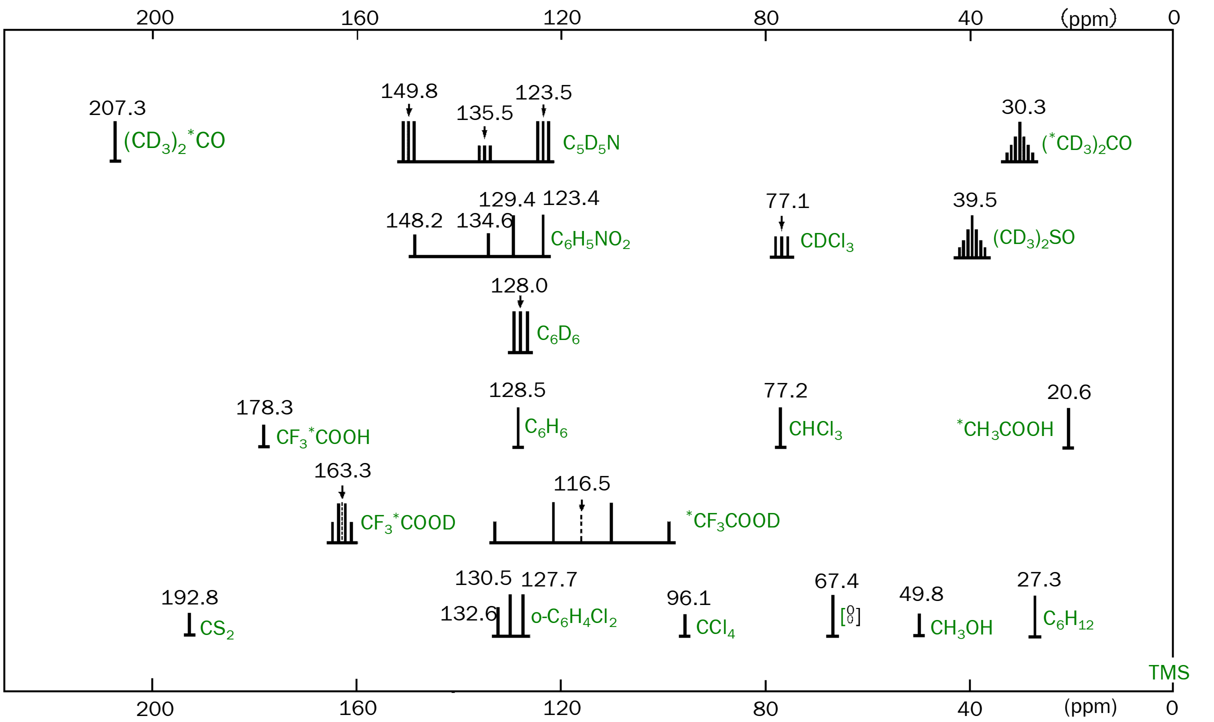

Figure 4.4 ^{13}C chemical shifts

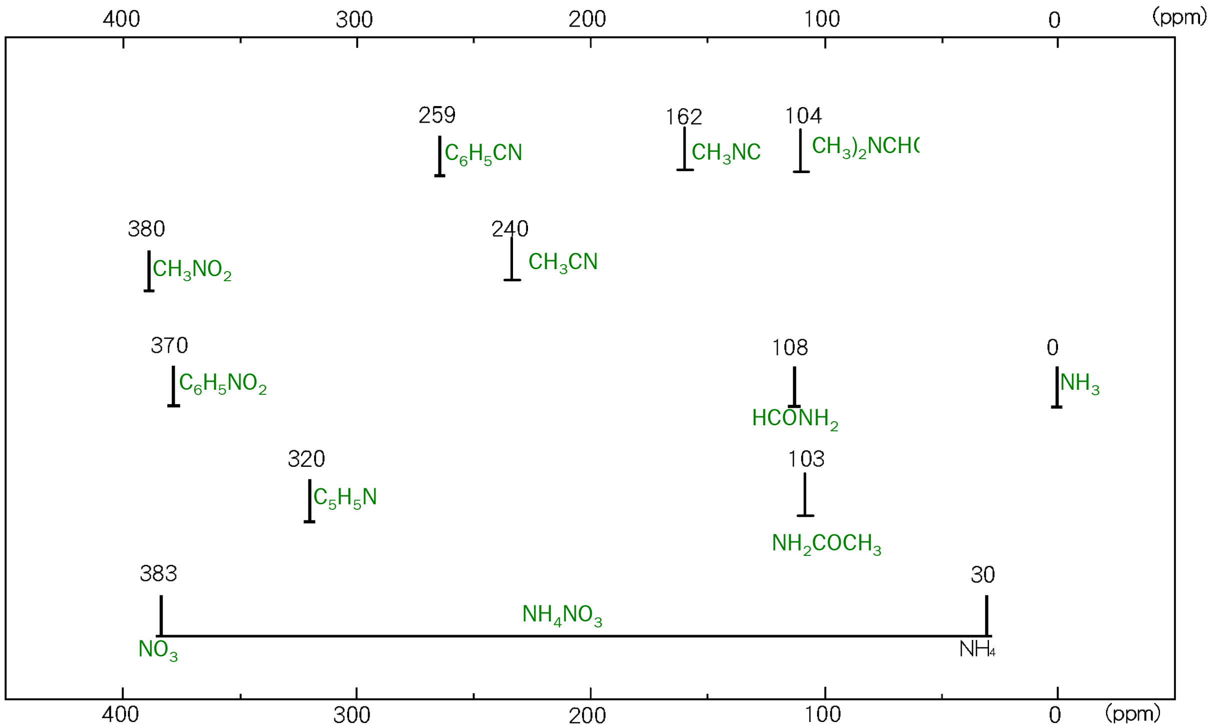

Figure 4.5 $^{14}N/^{15}N$ chemical shifts

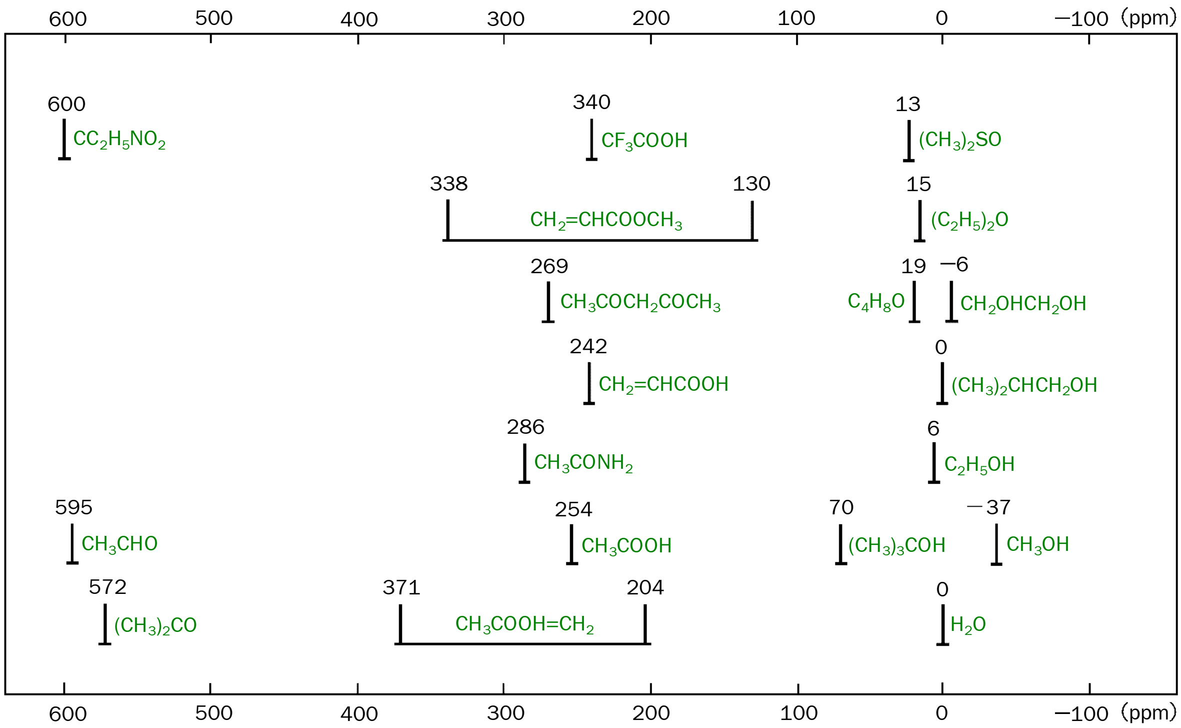

Figure 4.6 ^{17}O chemical shifts

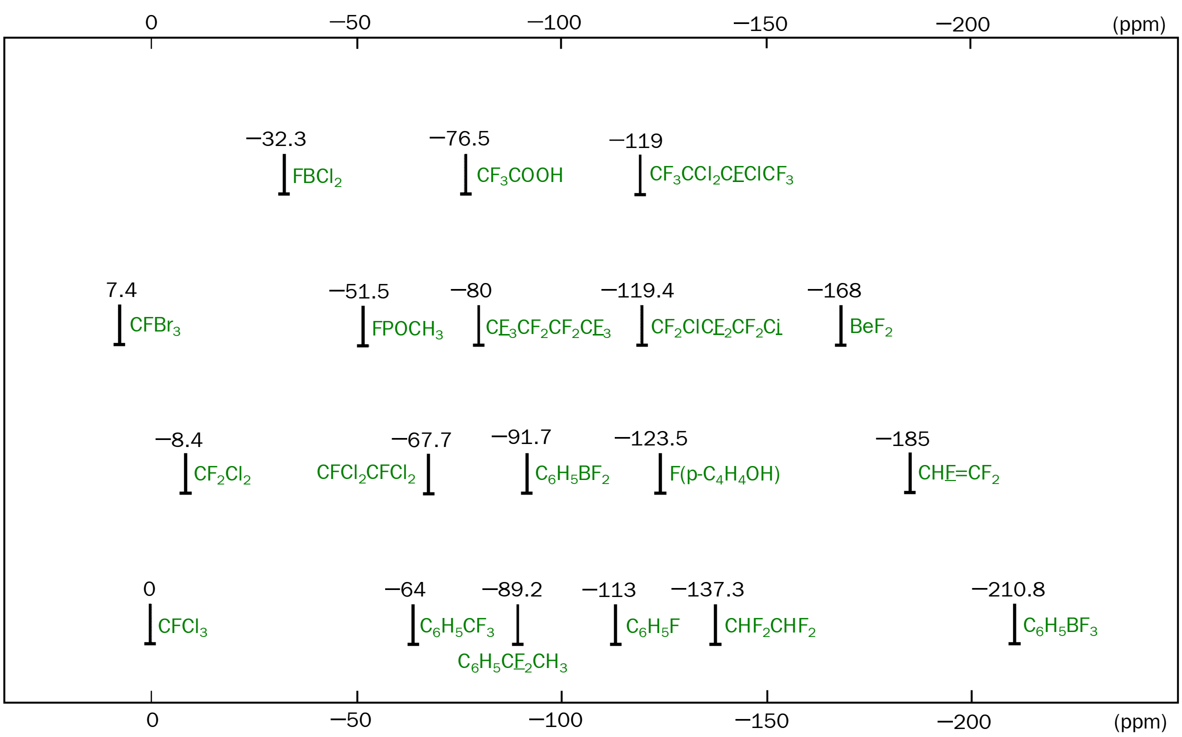

Figure 4.7 ^{19}F chemical shifts

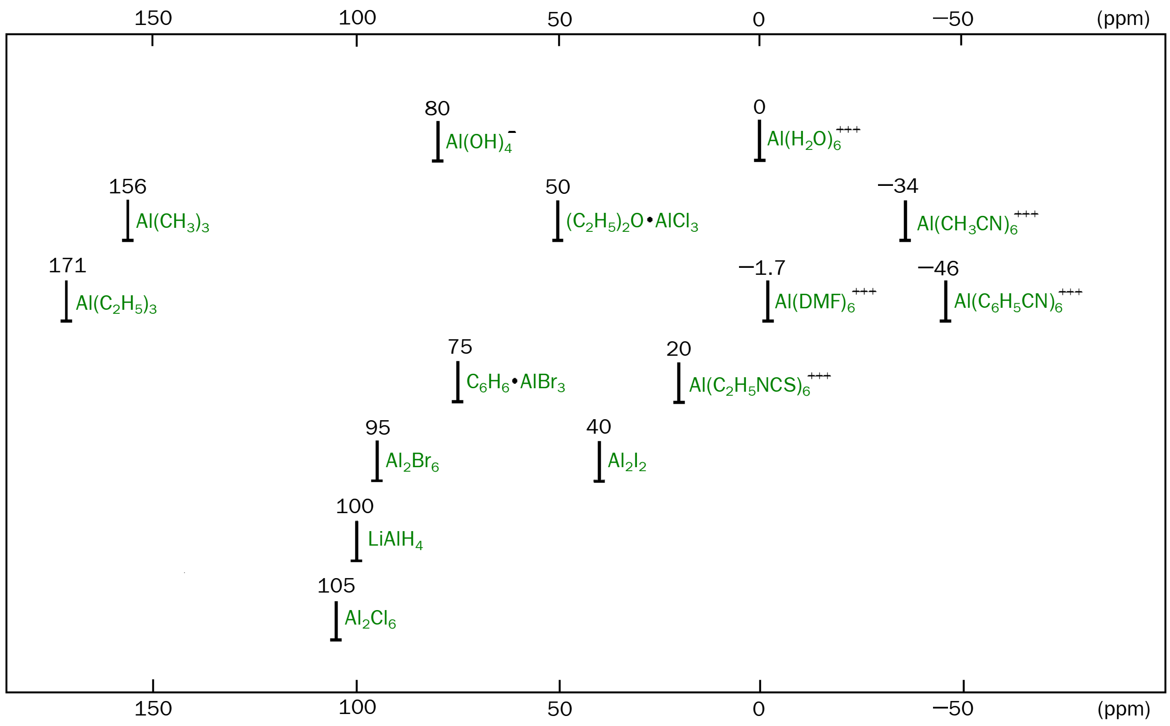

Figure 4.8 ^{27}Al chemical shifts

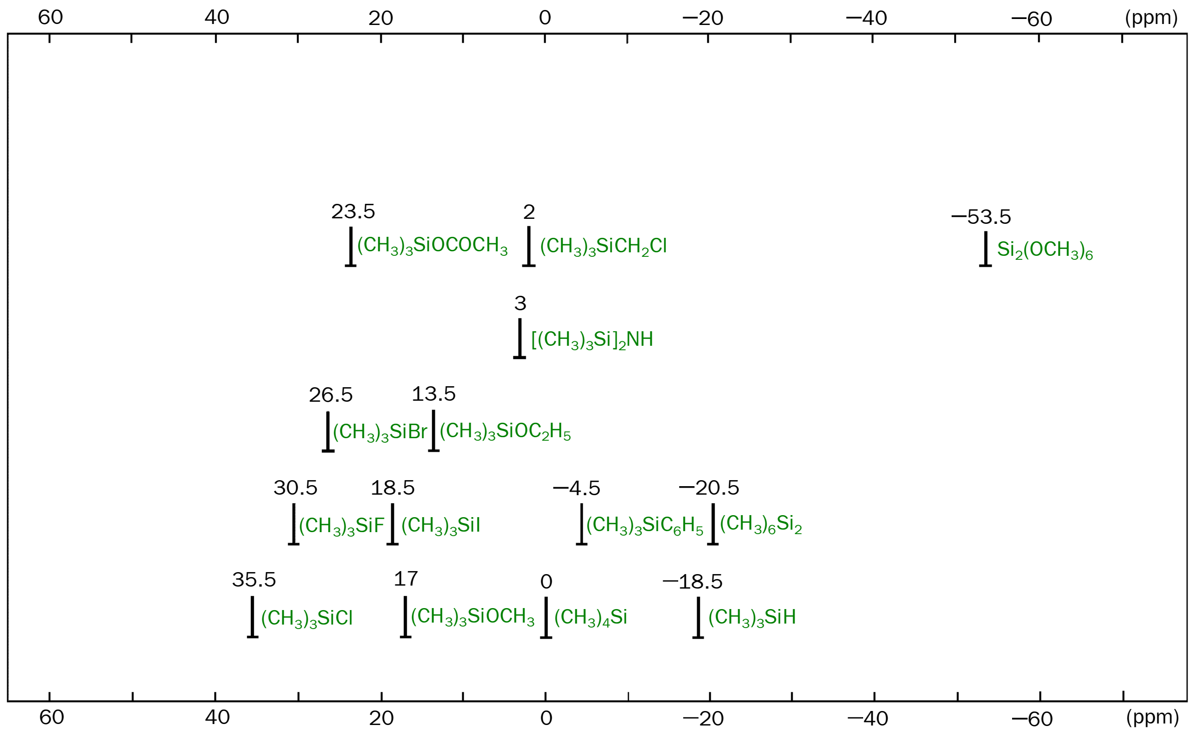

Figure 4.9 ^{29}Si chemical shifts

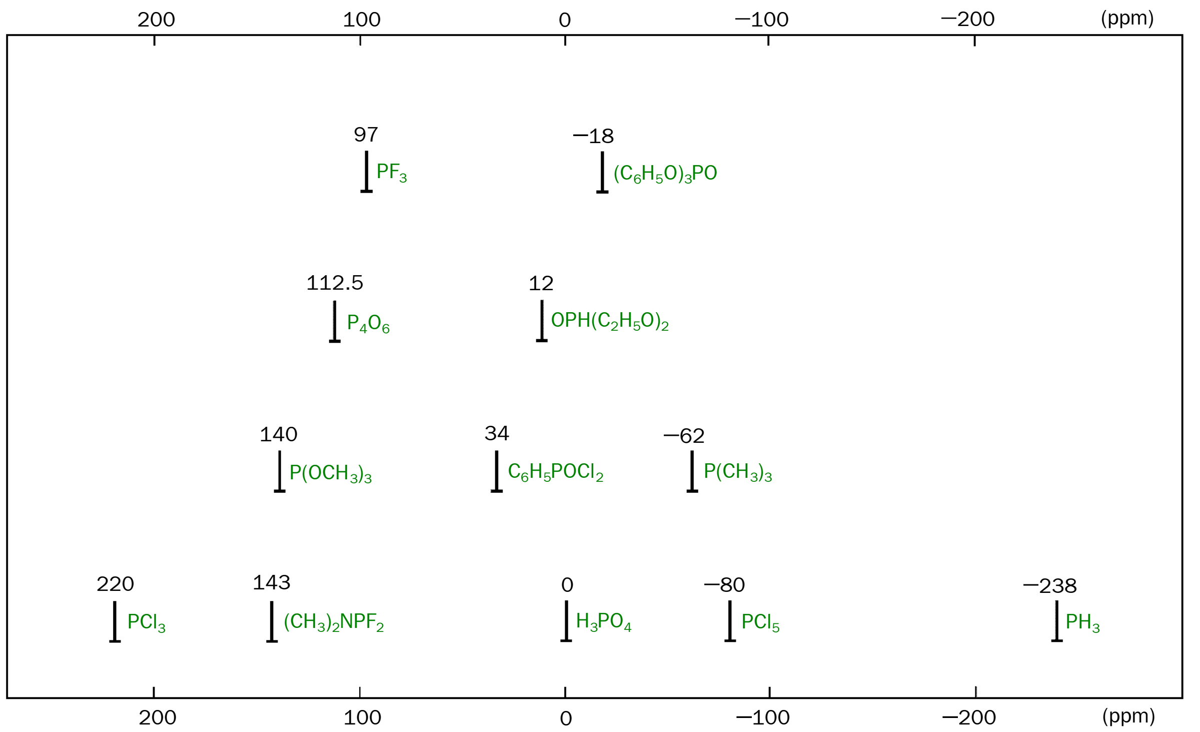

Figure 4.10 ^{31}P chemical shifts

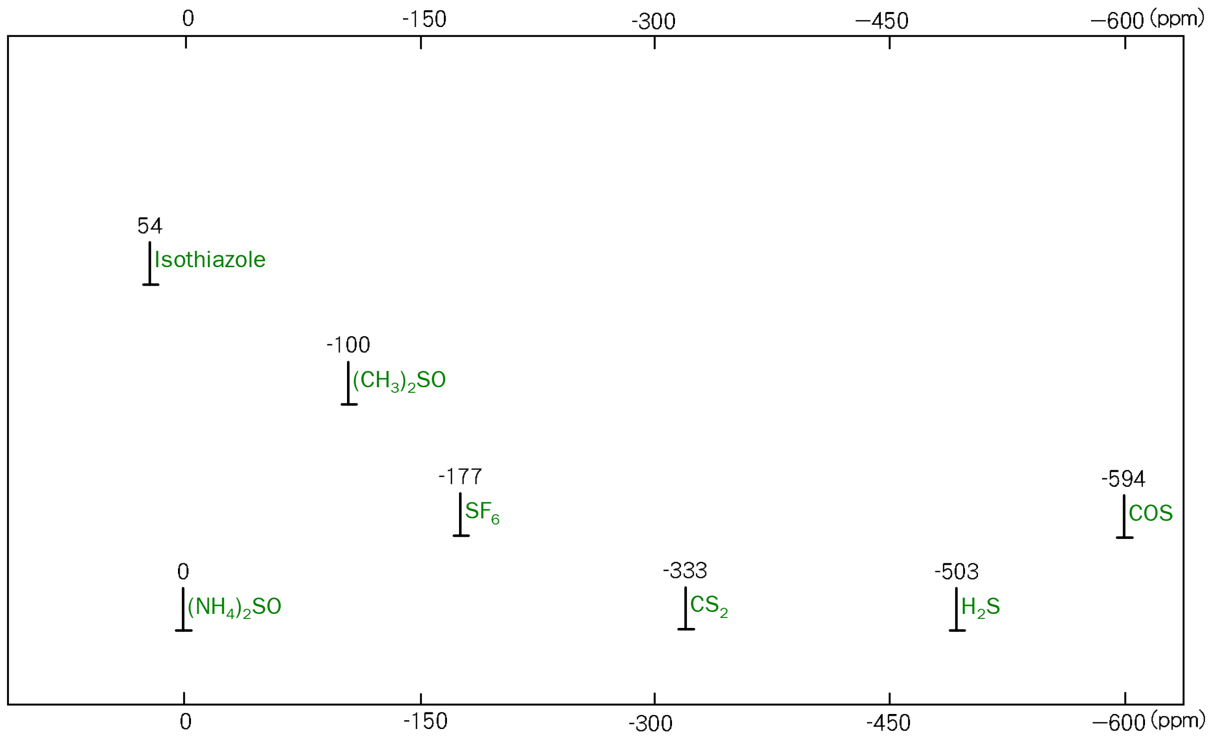

Figure 4.11 ^{33}S chemical shifts

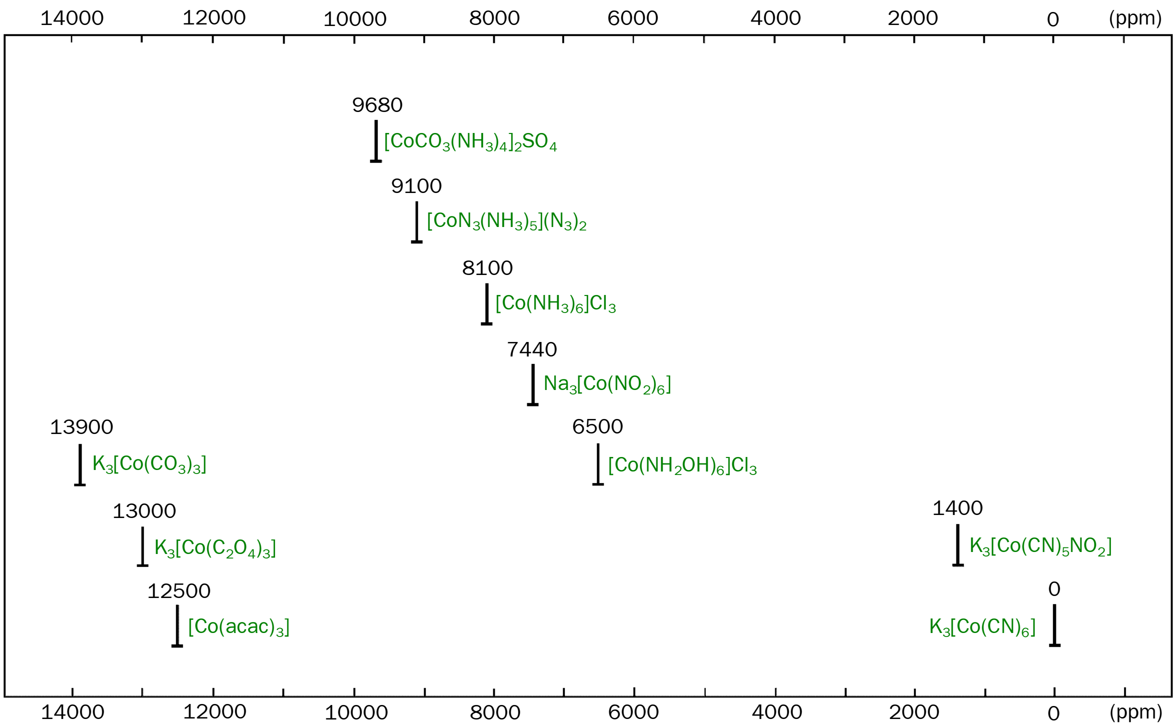

Figure 4.12 ^{59}Co chemical shifts

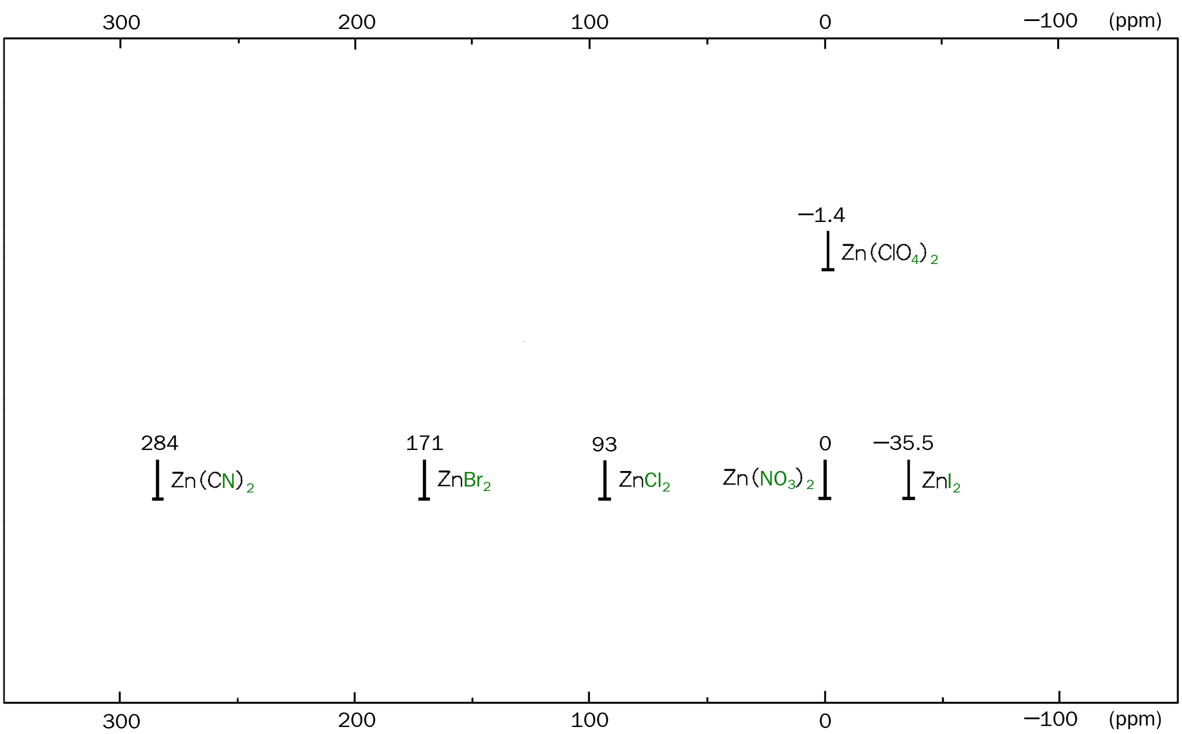

Figure 4.13 ^{67}Zn chemical shifts

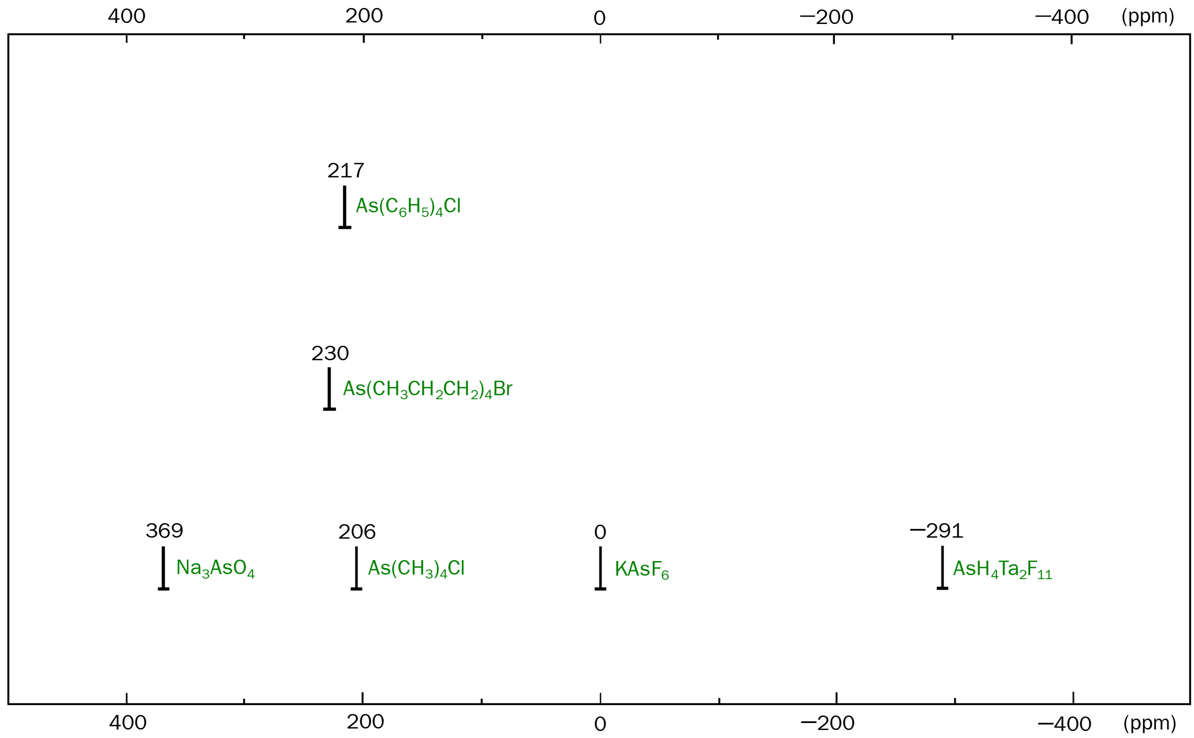

Figure 4.14 ^{75}As chemical shifts

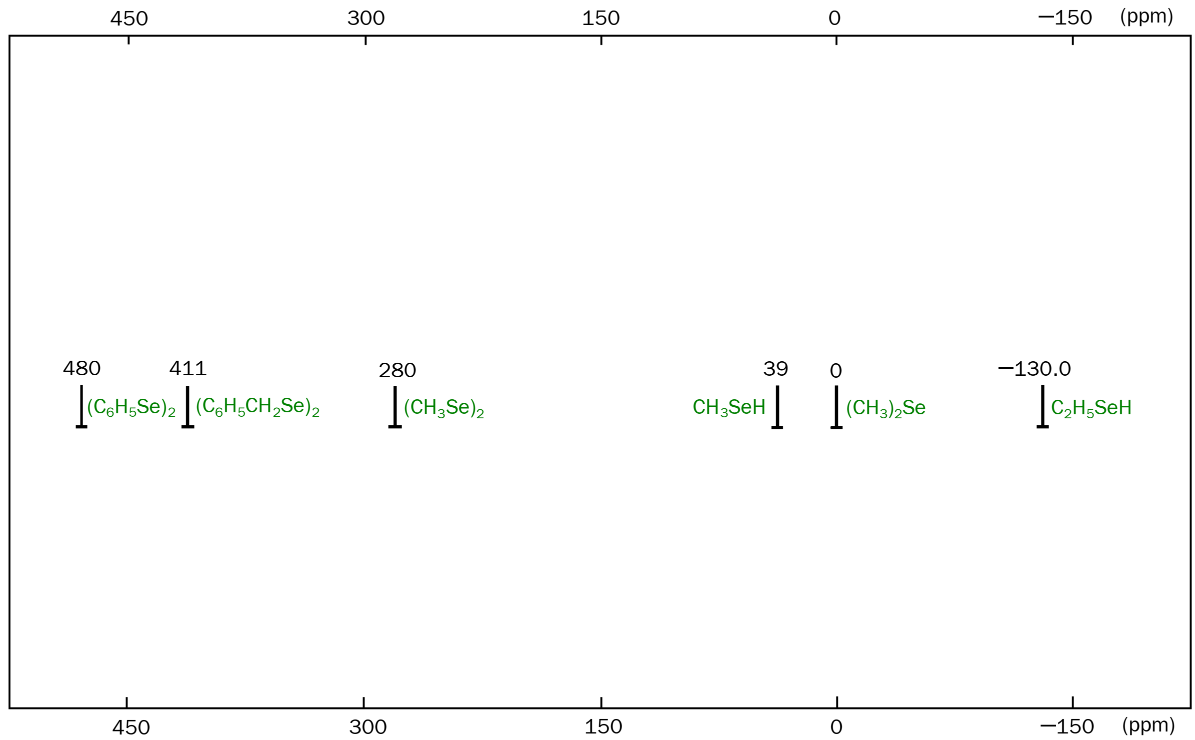

Figure 4.15 ^{77}Se chemical shifts

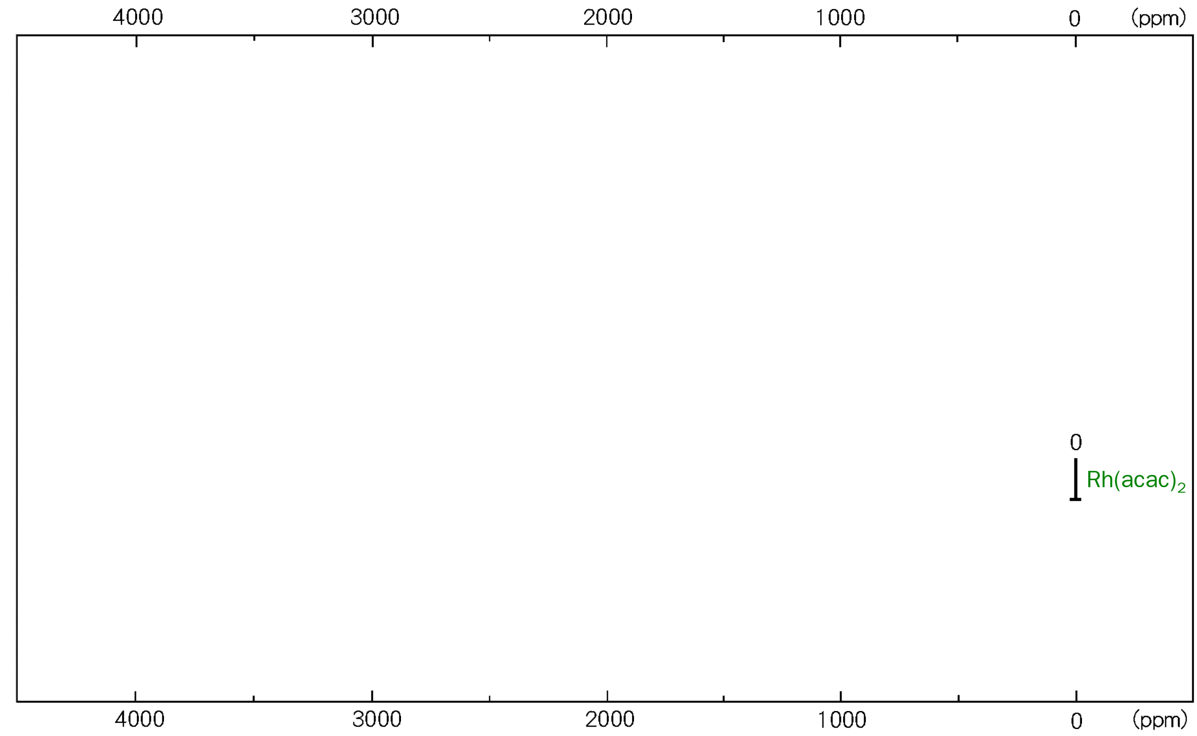

Figure 4.16 ^{103}Rh chemical shifts

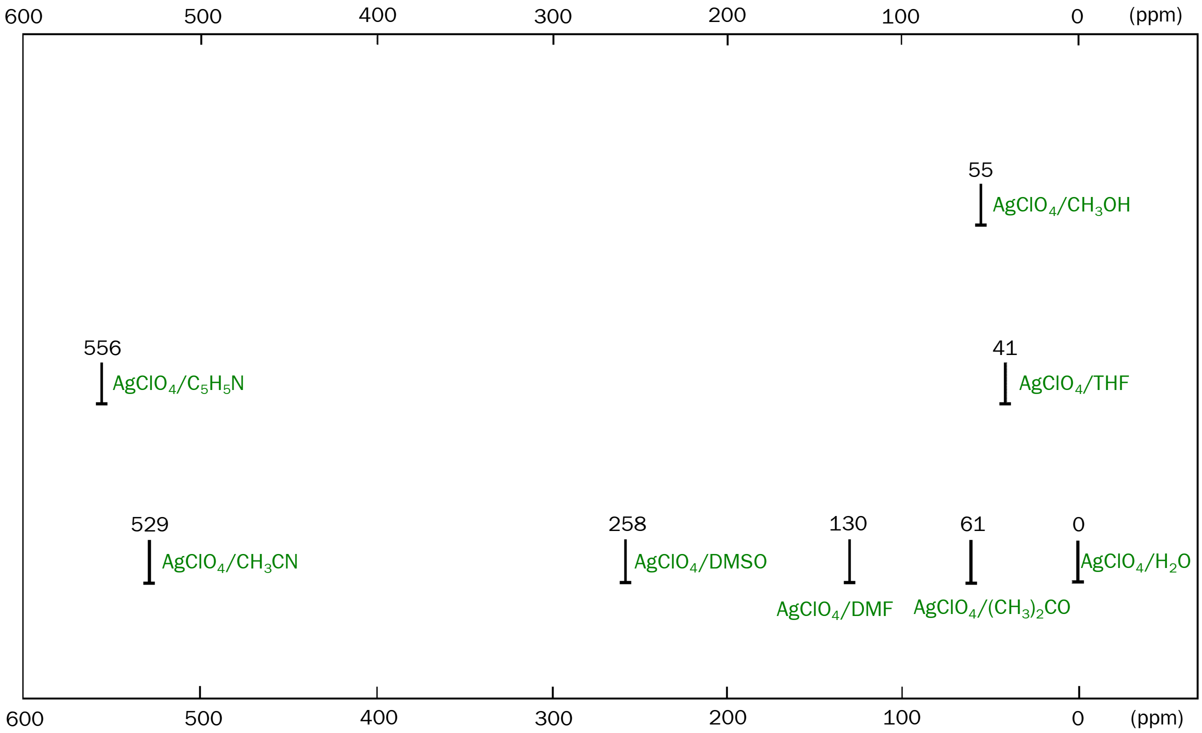

Figure 4.17 ^{109}Ag chemical shifts

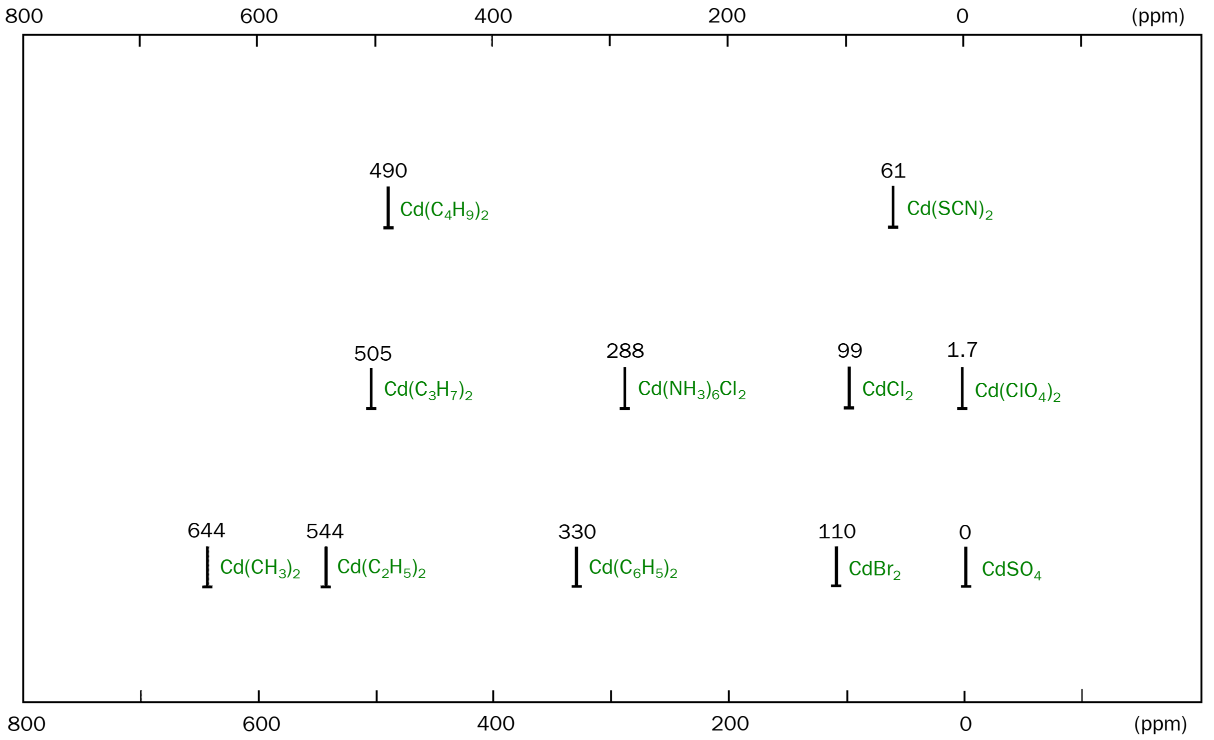

Figure 4.18 ^{113}Cd chemical shifts

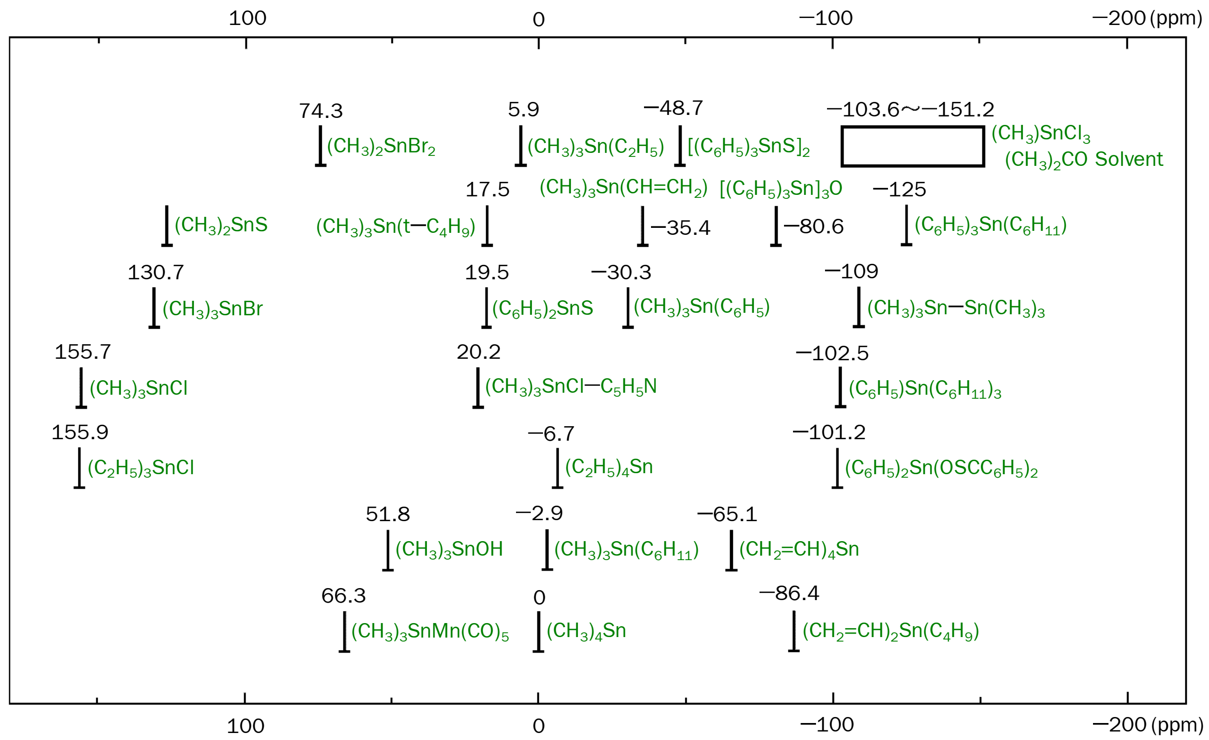

Figure 4.19 ^{119}Sn chemical shifts

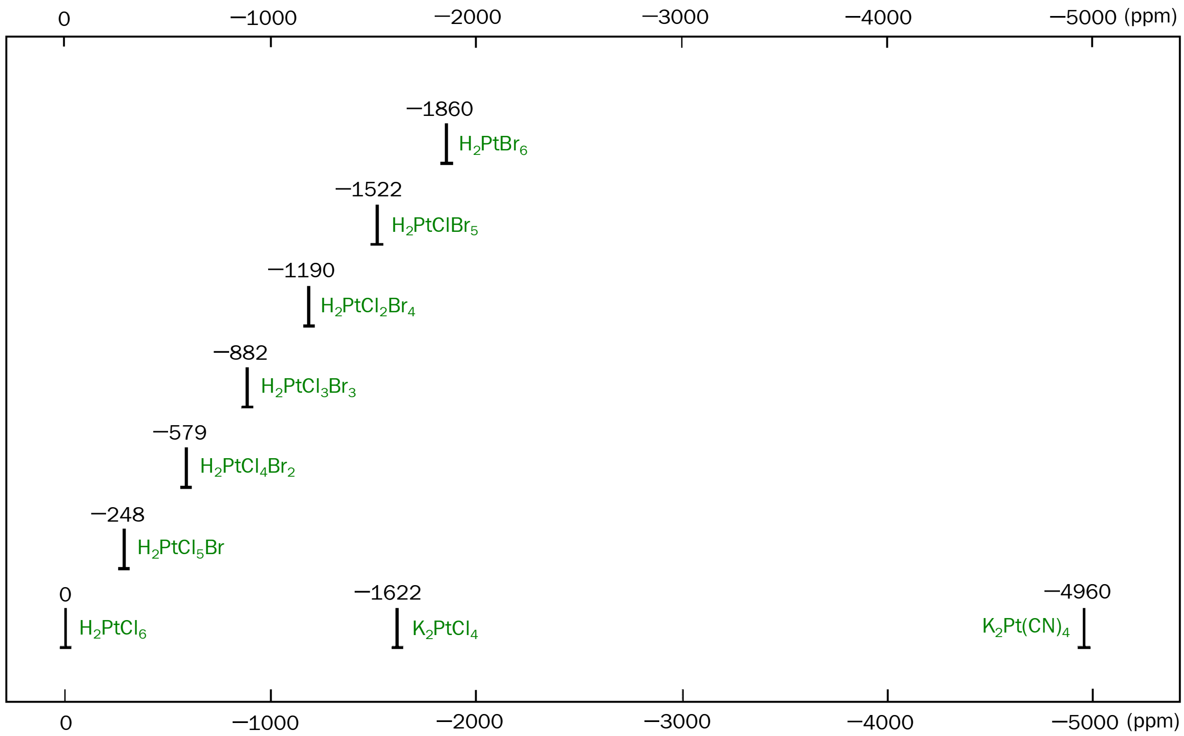

Figure 4.20 ^{195}Pt chemical shifts

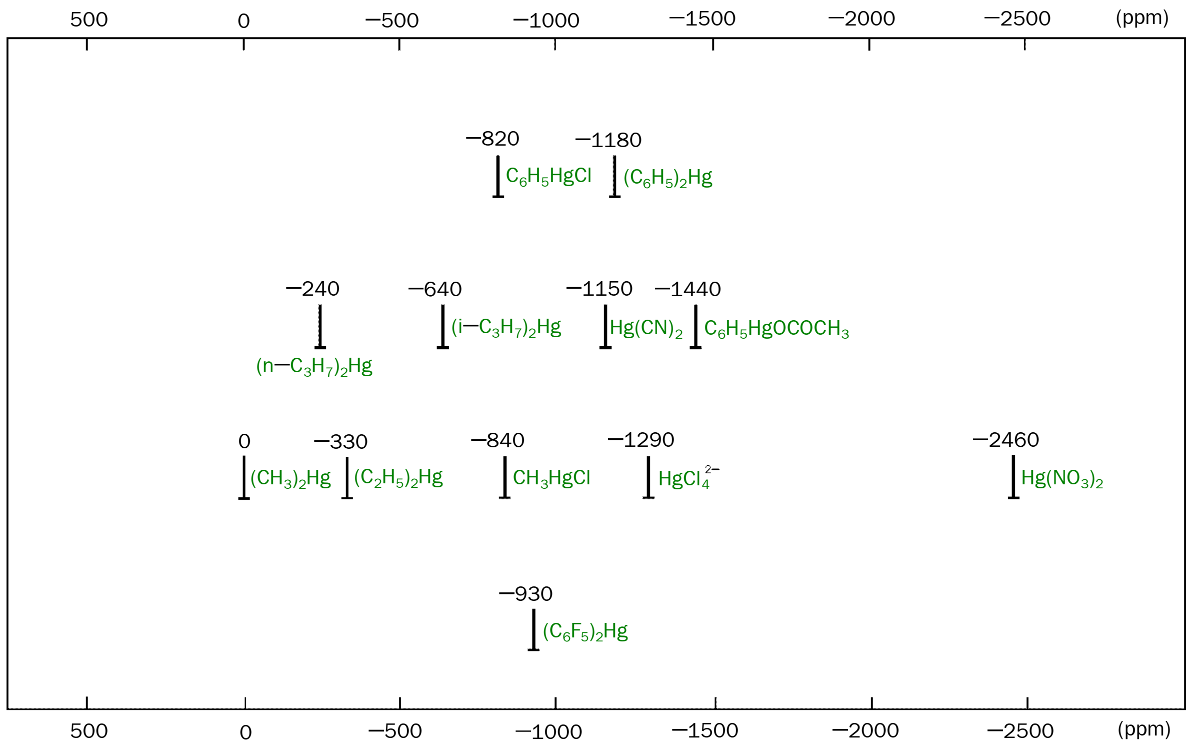

Figure 4.21 ^{199}Hg chemical shifts

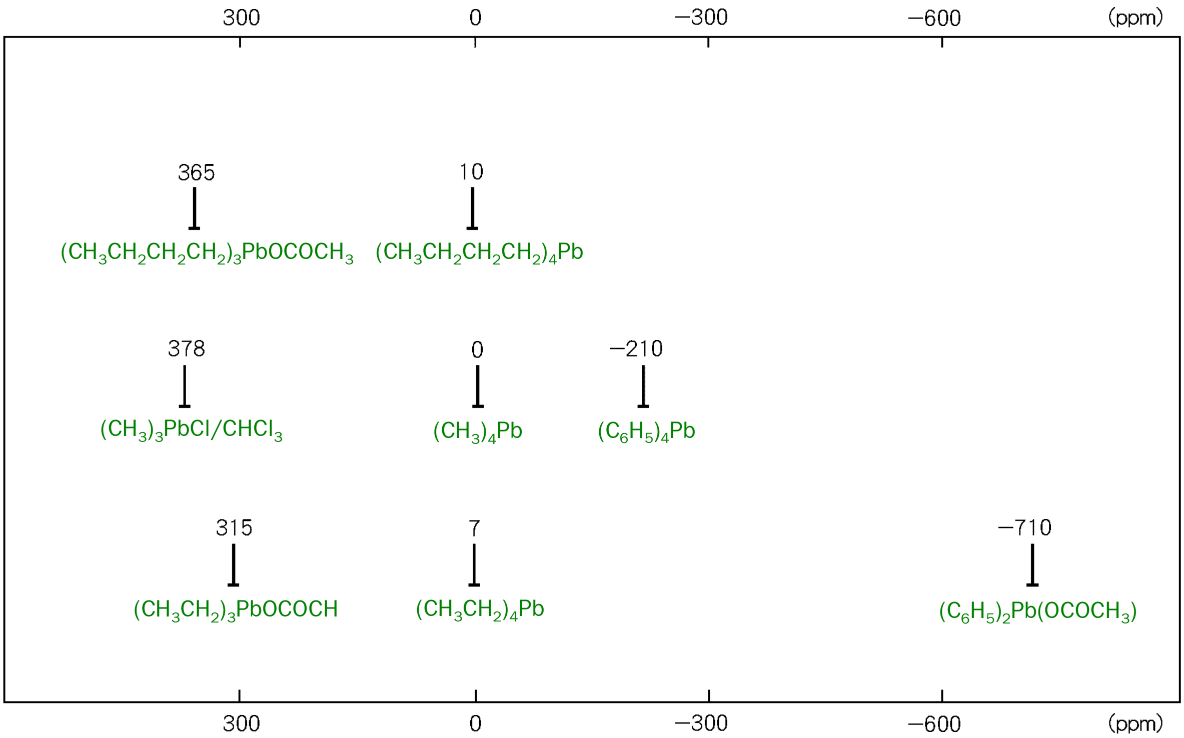

Figure 4.22 ^{207}Pb chemical shifts