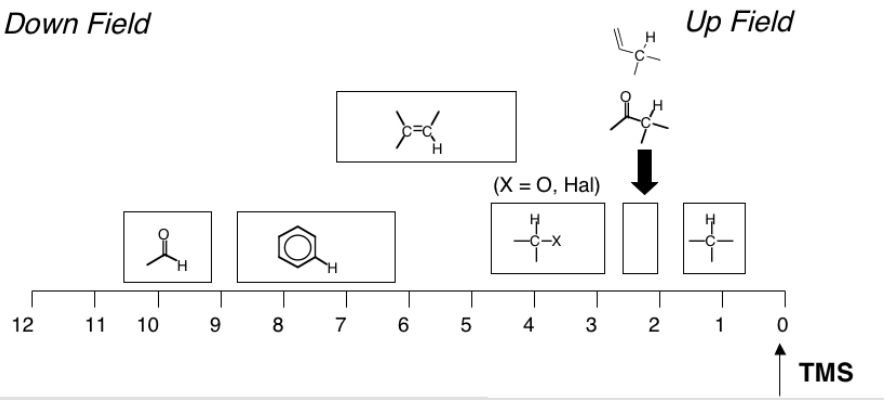
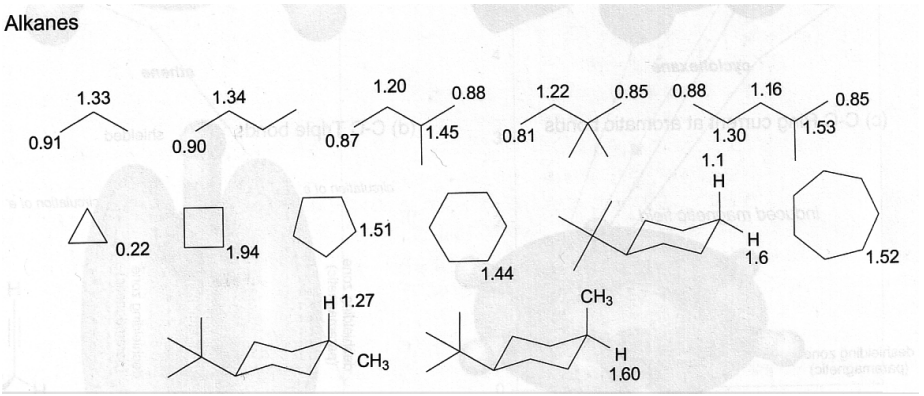
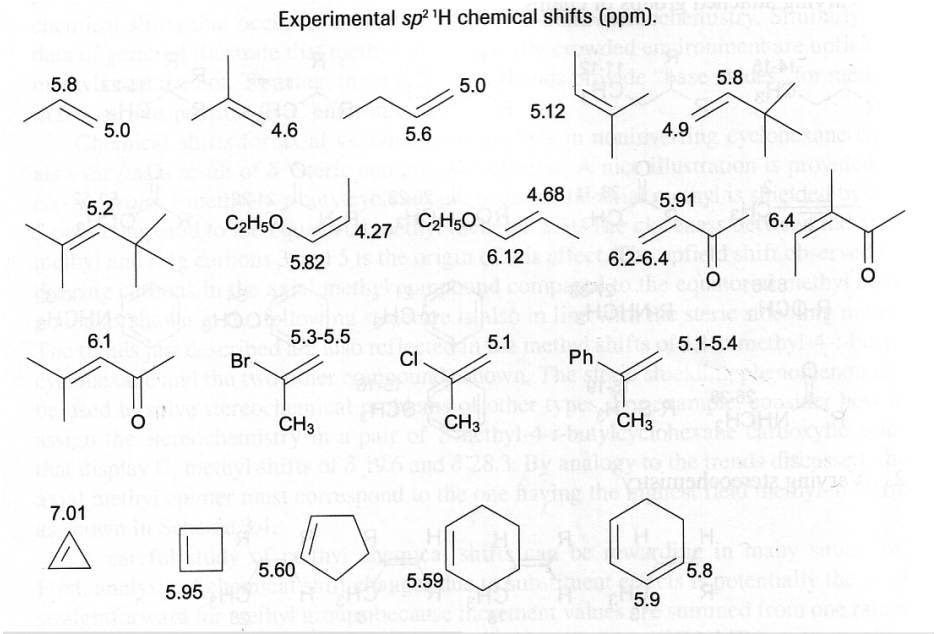
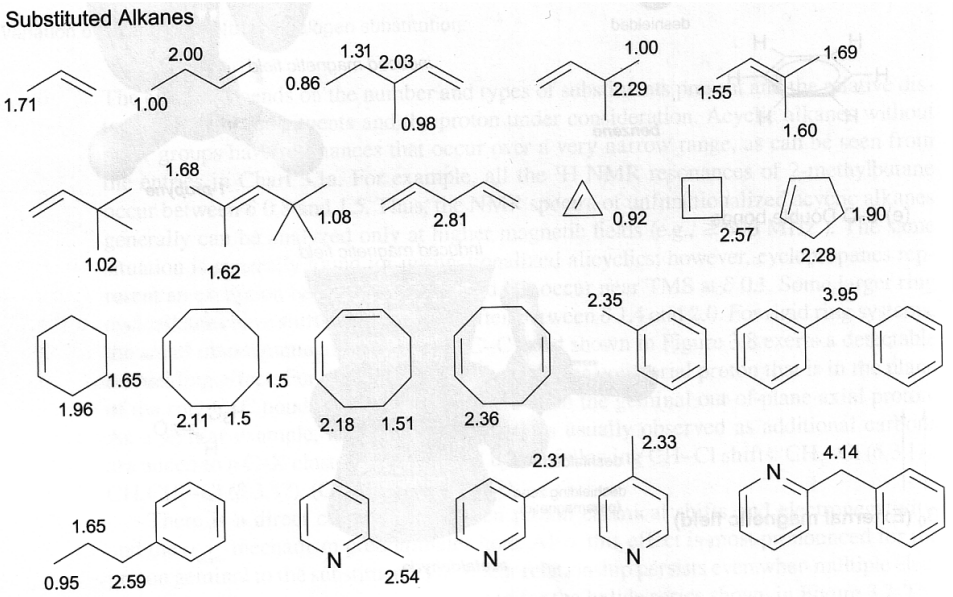
Overview of *typical* ^{1}H NMR shifts



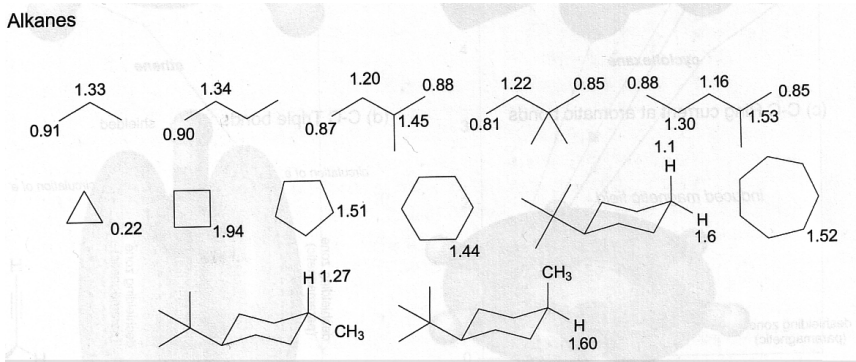


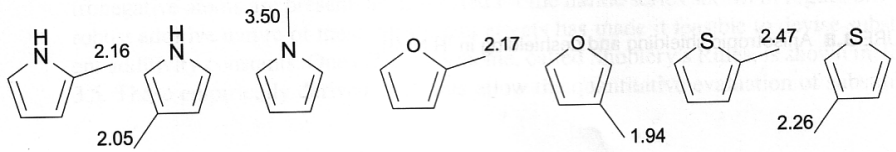
^{1}H NMR Tables



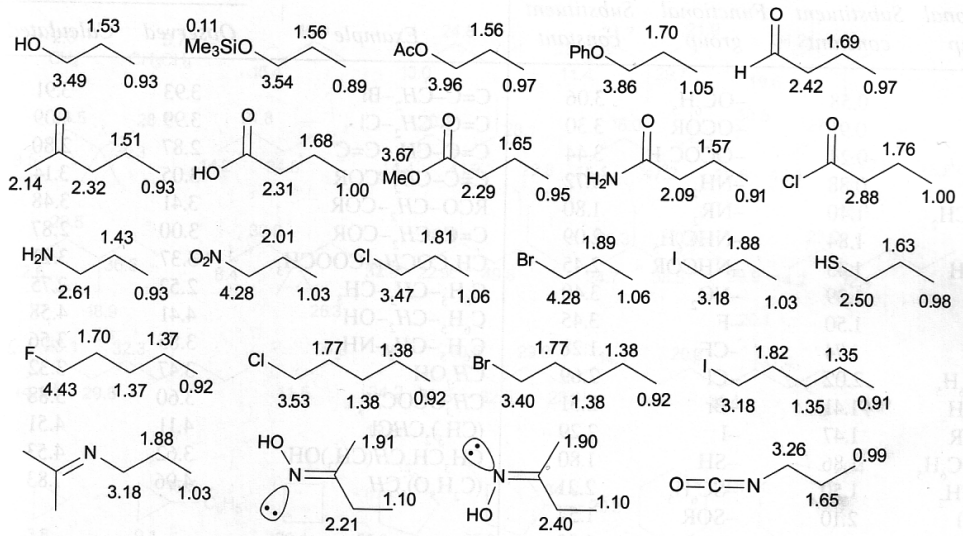


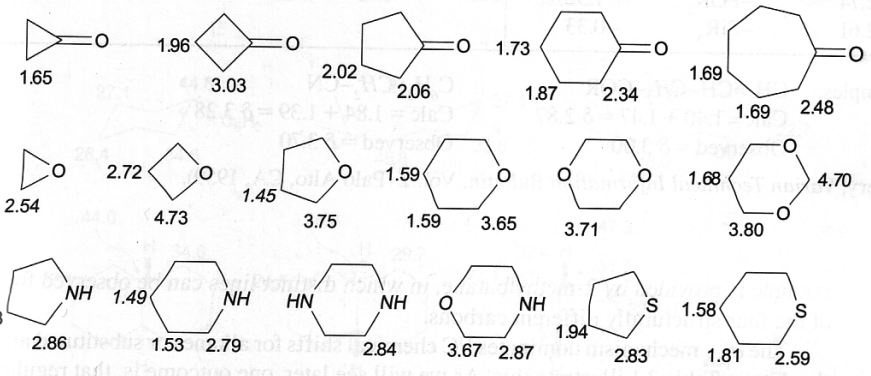
Alkanes





Functionalized Alkanes





Substituted Alkynes and C≡N

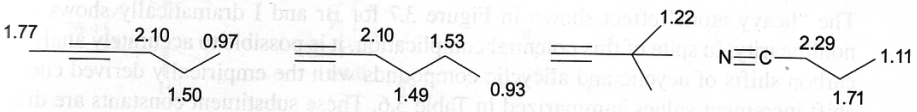


Table 13.1 Chemical Shifts of Protons on a Carbon Atom Adjacent (α Position) to a Functional Group in Aliphatic Compounds (M—Y)

▮ M = methyl
▪ M = methylene
▪ M = methine

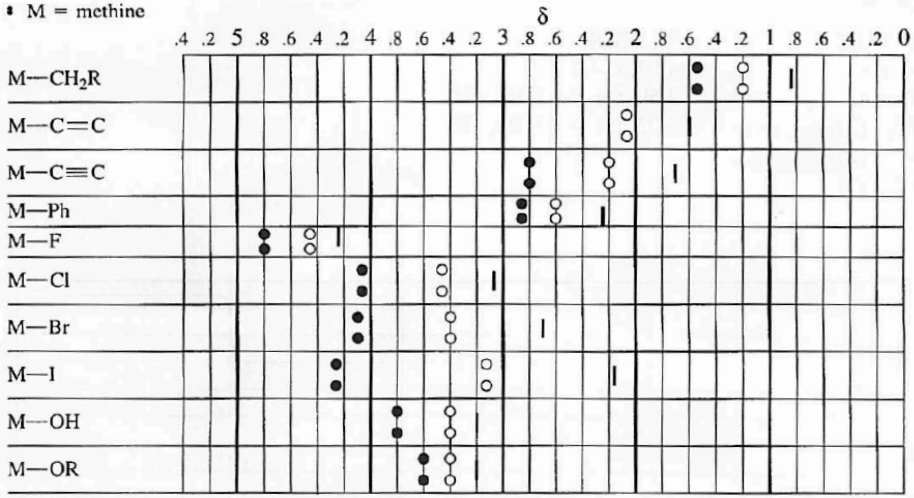
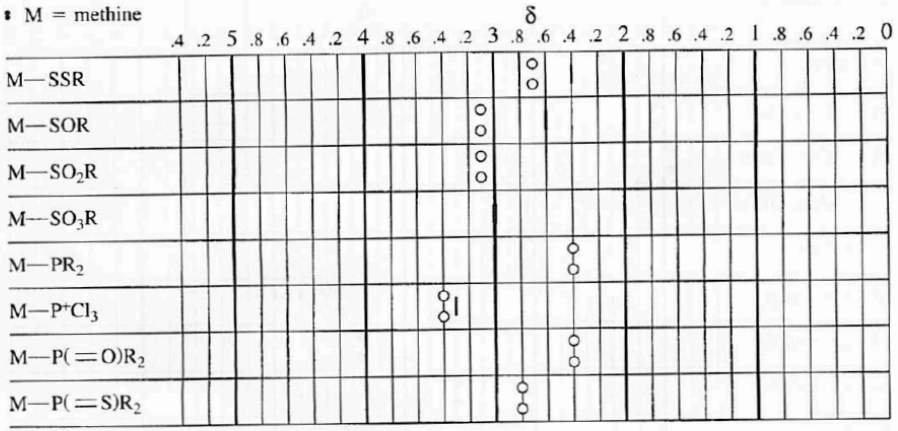


Table 13.1 (Continued)

▮ M = methyl
▪ M = methylene
▪ M = methine



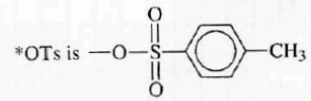
*OTs is 

Table 13.1 (Continued)

▮ M = methyl
▪ M = methylene
▪ M = methine

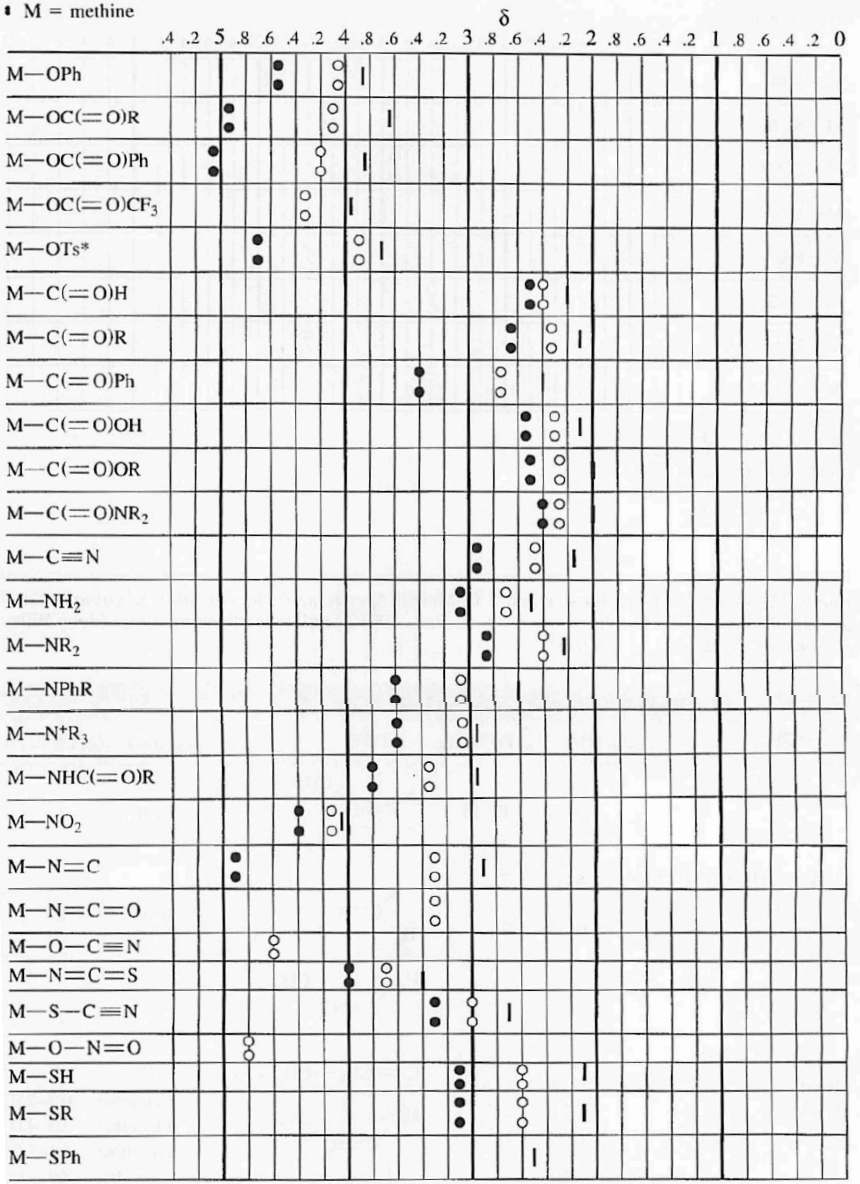
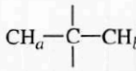
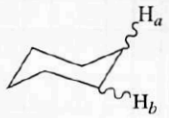
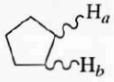


Table 13.2 Proton Spin-Coupling Constants

TYPE	J_{ab} (Hz)	J_{ab} TYPICAL
	0–30	12–15
$CH_a—CH_b$ (free rotaion)	6–8	7
	0–1	0
		
ax–ax	6–14	8–10
ax–eq	0–5	2–3
eq–eq	0–5	2–3
 (cis or trans)	*cis* 5–10 *trans* 5–10	

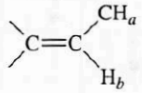
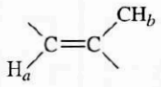
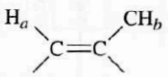
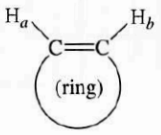
TYPE	J_{ab} (Hz)	J_{ab} TYPICAL
	4–10	7
	0–3	1.5
	0–3	2
$C{=}CH_a—CH_b{=}C$	9–13	10
	3 member 4 member 5 member 6 member 7 member 8 member	0.5–2.0 2.5–4.0 5.1–7.0 8.8–11.0 9–13 10–13

Table 13.3 Chemical Shifts in Alicyclic Rings

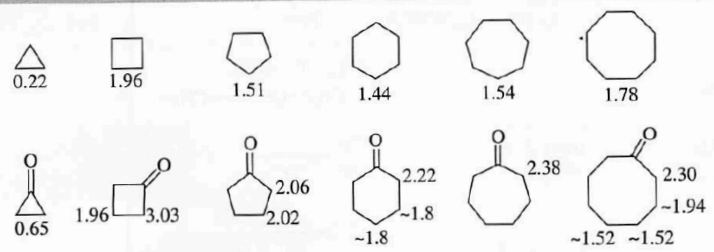
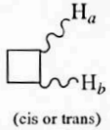
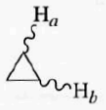
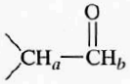
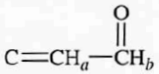
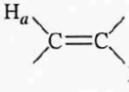
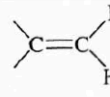
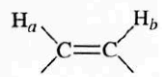
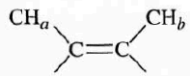
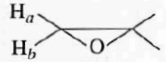
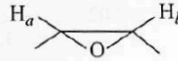
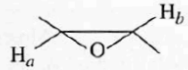
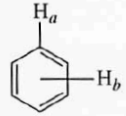
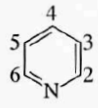
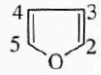
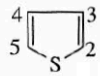


Table 14.3 Chemical Shifts of Alkyne Protons

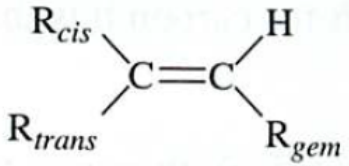
HC≡CR	1.73–1.88
HC≡C—COH	2.23
HC≡C—C≡CR	1.95
HC≡CH	1.80
HC≡CAR	2.71–3.37
HC≡C—C≡CR	2.60–3.10

Table 13.2 (Continued)

TYPE	J_{ab} (Hz)	J_{ab} TYPICAL
 (cis or trans)	*cis* 4–12 *trans* 2–10	
 (cis or trans)	*cis* 7–13 *trans* 4–9	
$CH_a—OH_b$ (no exchange)	4–10	5
	1–3	2–3
	5–8	6
	12–18	17
	0–3	0–2
	6–12	10
	0–3	1–2

TYPE	J_{ab} (Hz)	J_{ab} TYPICAL
$CH_a—C{\equiv}CH_b$	2–3	
$—CH_a—C{\equiv}C—CH_b—$	2–3	
		6
		4
		2.5
	*J* (ortho) 6–10 *J* (meta) 1–3 *J* (para) 0–1	9 3 ~0
	*J* (2–3) (5–6) *J* (3–4) (7–9) *J* (2–4) (1–2) *J* (3–5) (1–2) *J* (2–5) (0–1) *J* (2–6) (0–1)	5 8 1.5 1.5 1 ~0
	*J* (2–3) 1.3–2.0 *J* (3–4) 3.1–3.8 *J* (2–4) 0–0 *J* (2–5) 1–2	1..8 3.6 ~0 1.5
	*J* (2–3) 4.9–6.2 *J* (3–4) 3.4–5.0 *J* (2–4) 1.2–1.7 *J* (2–5) 3.2–3.7	5.4 4.0 1.5 3.4

CALCULATING THE ^{1}H NMR CHEMICAL SHIFTS OF ALKENES



$$\delta_H = 5.25 + Z_{gem} + Z_{cis} + Z_{trans}$$

FROM TABLE 14.4 (LABBOOK)
OR TABLE H.6 (SPEC BOOK)

Table 14.4 Calculation of ^{1}H NMR Chemical Shifts for Alkenes

See Figure 14.12 for more information.

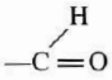
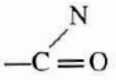
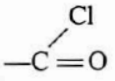
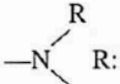
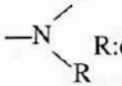
	Z				Z		
SUBSTITUENT R	GEM	CIS	TRANS	SUBSTITUENT R	GEM	CIS	TRANS
—H	0	0	0		1.03	0.97	1.21
—Alkyl	0.44	−0.26	−0.29				
—Alkyl-ring[a]	0.71	−0.33	−0.30				
—CH_2O, —CH_2I	0.67	−0.02	−0.07		1.37	0.93	0.35
—CH_2S	0.53	−0.15	−0.15				
—CH_2Cl, —CH_2Br	0.72	0.12	0.07				
—CH_2N	0.66	−0.05	−0.23		1.10	1.41	0.99
—C≡C	0.50	0.35	0.10	—OR, R:aliph	1.18	−1.06	−1.28
—C≡N	0.23	0.78	0.58	—OR, R:conj[b]	1.14	−0.65	−1.05
—C=C	0.98	−0.04	−0.21	—OCOR	2.09	−0.40	−0.67
—C=C conj[b]	1.26	0.08	−0.01	—Aromatic	1.35	0.37	−0.10
—C=O	1.10	1.13	0.81	—Cl	1.00	0.19	0.03
—C=O conj[b]	1.06	1.01	0.95	—Br	1.04	0.40	0.55
—COOH	1.00	1.35	0.74	 R: aliph	0.69	−1.19	−1.31
—COOH conj[b]	0.69	0.97	0.39				
—COOR	0.84	1.15	0.56	 R:conj[b]	2.30	−0.73	−0.81
—COOR conj[b]	0.68	1.02	0.33				
				—SR	1.00	−0.24	−0.04
				—SO_2	1.58	1.15	0.95

Table 14.5 Incremental Shifts of the Aromatic Carbon Atoms of Monosubstituted Benzenes (ppm from Benzene at 128.5 ppm, + downfield, − upfield). Carbon Atom of Substituents in parts per million from TMS[a]

SUBSTITUENT	C-1 (ATTACHMENT)	C-2	C-3	C-4	C OF SUBSTITUENT (ppm from TMS)
H	0.0	0.0	0.0	0.0	
CH_3	9.3	+0.7	−0.1	−2.9	21.3
CH_2CH_3	+15.6	−0.5	0.0	−2.6	29.2 (CH_2), 15.8 (CH_3)
$CH(CH_3)_2$	+20.1	−2.0	0.0	−2.5	34.4 (CH), 24.1 (CH_3)
$C(CH_3)_3$	+22.2	−3.4	−0.4	−3.1	34.5 (C), 31.4 (CH_3)
$CH{=}CH_2$	+9.1	−2.4	+0.2	−0.5	137.1 (CH), 113.3 (CH_2)
$C{\equiv}CH$	−5.8	+6.9	+0.1	+0.4	84.0 (C), 77.8 (CH)
C_6H_5	+12.1	−1.8	−0.1	−1.6	
CH_2OH	+13.3	−0.8	−0.6	−0.4	64.5
CH_2OCCH_3 (O)	+7.7	~0.0	~0.0	~0.0	20.7 (CH_3), 66.1 (CH_2), 170.5 (C=O)
OH	+26.6	−12.7	+1.6	−7.3	
OCH_3	+31.4	−14.4	+1.0	−7.7	54.1
OC_6H_5	+29.0	−9.4	+1.6	−5.3	
$OCCH_3$ (O)	+22.4	−7.1	−0.4	−3.2	23.9 (CH_3), 169.7 (C=O)
CH (O)	+8.2	+1.2	+0.6	+5.8	192.0
CCH_3 (O)	+7.8	−0.4	−0.4	+2.8	24.6 (CH_3), 195.7 (C=O)
CC_6H_5 (O)	+9.1	+1.5	−0.2	+3.8	196.4 (C=O)
CCF_3 (O)	−5.6	+1.8	+0.7	+6.7	
COH (O)	+2.9	+1.3	+0.4	+4.3	168.0
$COCH_3$ (O)	+2.0	+1.2	−0.1	+4.8	51.0 (CH_3), 166.8 (C=O)
CCl (O)	+4.6	+2.9	+0.6	+7.0	168.5
$C{\equiv}N$	−16.0	+3.6	+0.6	+4.3	119.5
NH_2	+19.2	−12.4	+1.3	−9.5	
$N(CH_3)_2$	+22.4	−15.7	+0.8	−11.8	40.3
$NHCCH_3$ (O)	+11.1	−9.9	+0.2	−5.6	

Table 14.5 (Continued)

SUBSTITUENT	C-1 (ATTACHMENT)	C-2	C-3	C-4	C OF SUBSTITUENT (ppm from TMS)
NO_2	+19.6	−5.3	+0.9	+6.0	
$N{=}C{=}O$	+5.7	−3.6	+1.2	−2.8	129.5
F	+35.1	−14.3	+0.9	−4.5	
Cl	+6.4	+0.2	+1.0	−2.0	
Br	−5.4	+3.4	+2.2	−1.0	
I	−32.2	+9.9	+2.6	−7.3	
CF_3	+2.6	−3.1	+0.4	+3.4	
SH	+2.3	+0.6	+0.2	−3.3	
SCH_3	+10.2	−1.8	+0.4	−3.6	15.9
SO_2NH_2	+15.3	−2.9	+0.4	+3.3	
$Si(CH_3)_3$	+13.4	+4.4	−1.1	−1.1	

Table 14.6 Chemical Shifts of Protons on Monosubstituted Benzene Rings