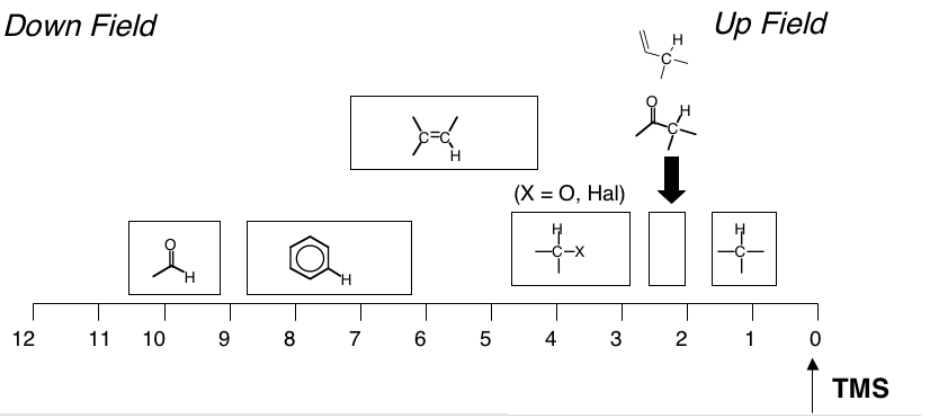
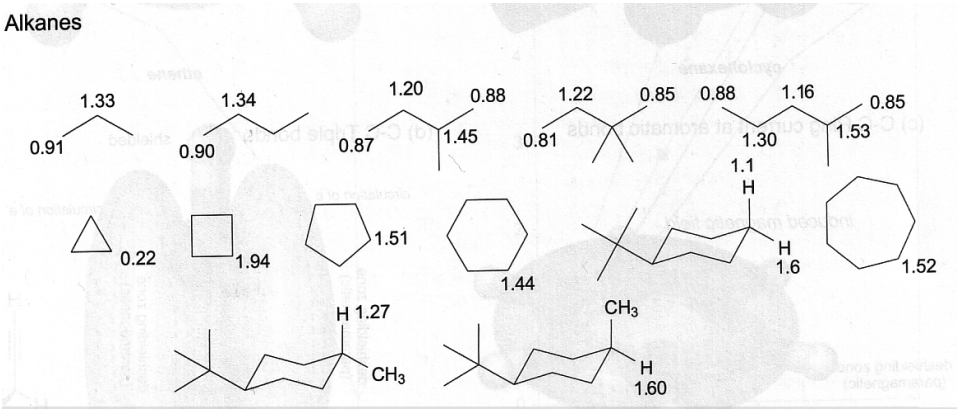
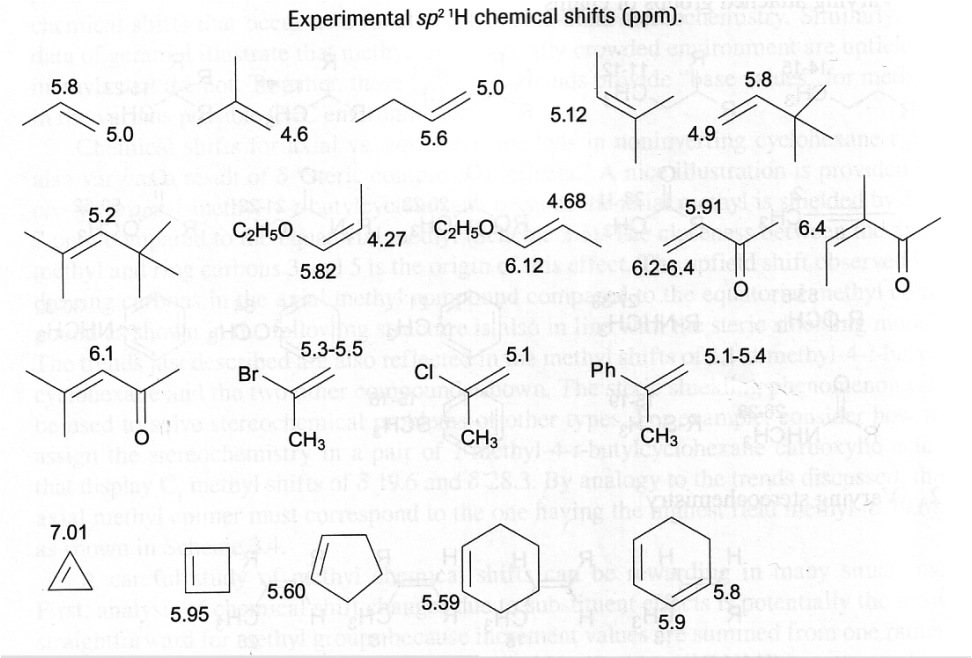
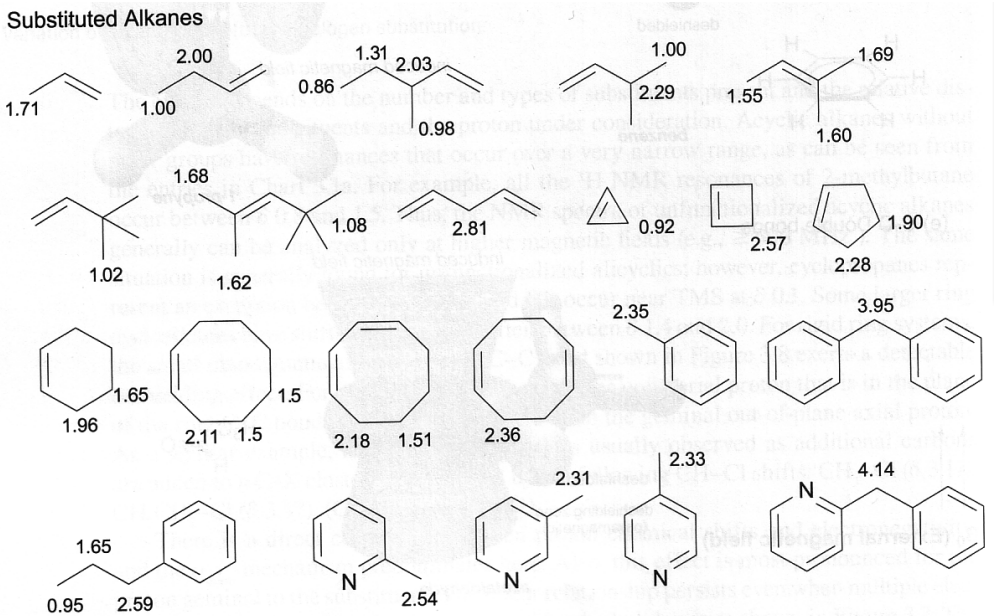
Overview of *typical* ^{1}H NMR shifts





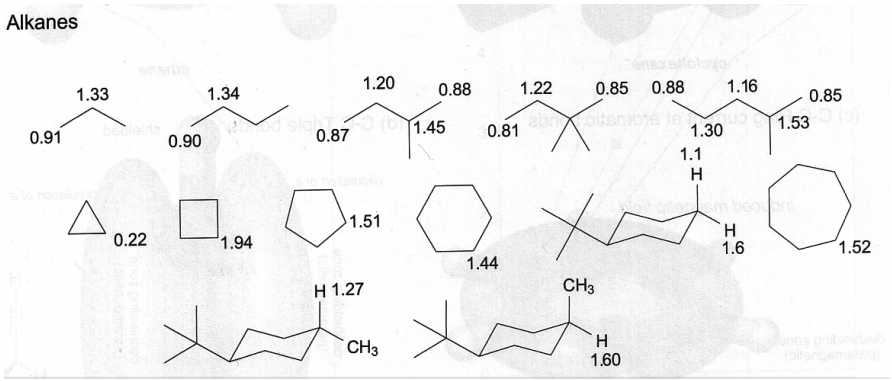
^{1}H NMR Tables

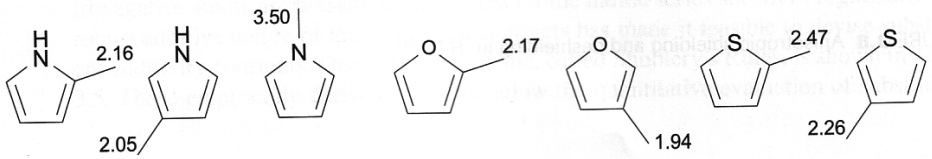




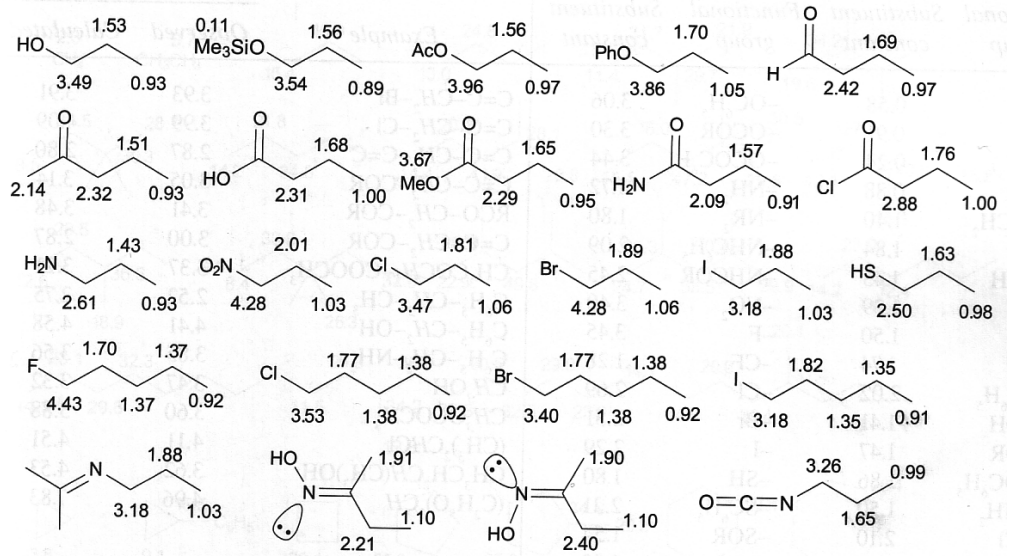
Experimental sp^3 ^{1}H chemical shifts (ppm) (*cont.*).

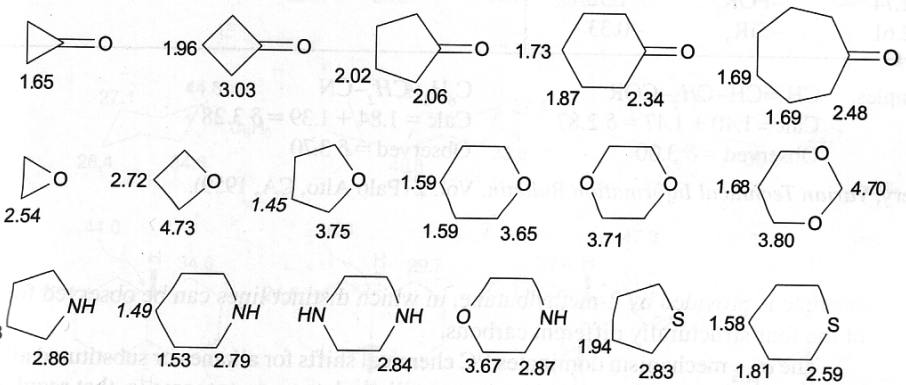
Alkanes





Functionalized Alkanes





Substituted Alkynes and C≡N

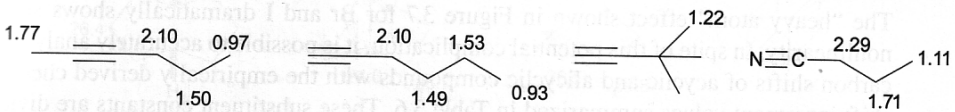


Table 13.1 Chemical Shifts of Protons on a Carbon Atom Adjacent (α Position) to a Functional Group in Aliphatic Compounds (M—Y)

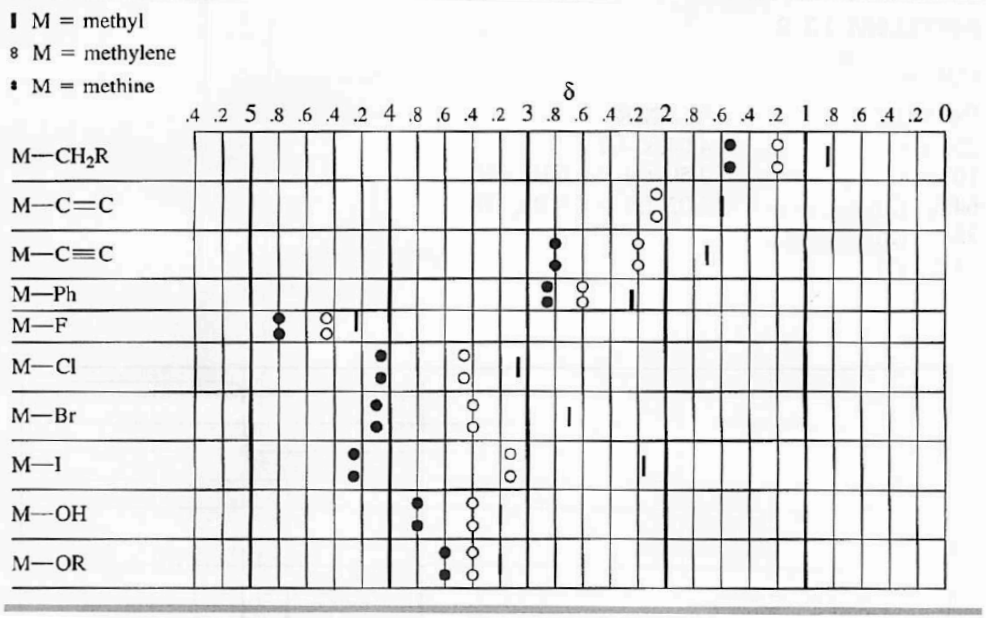
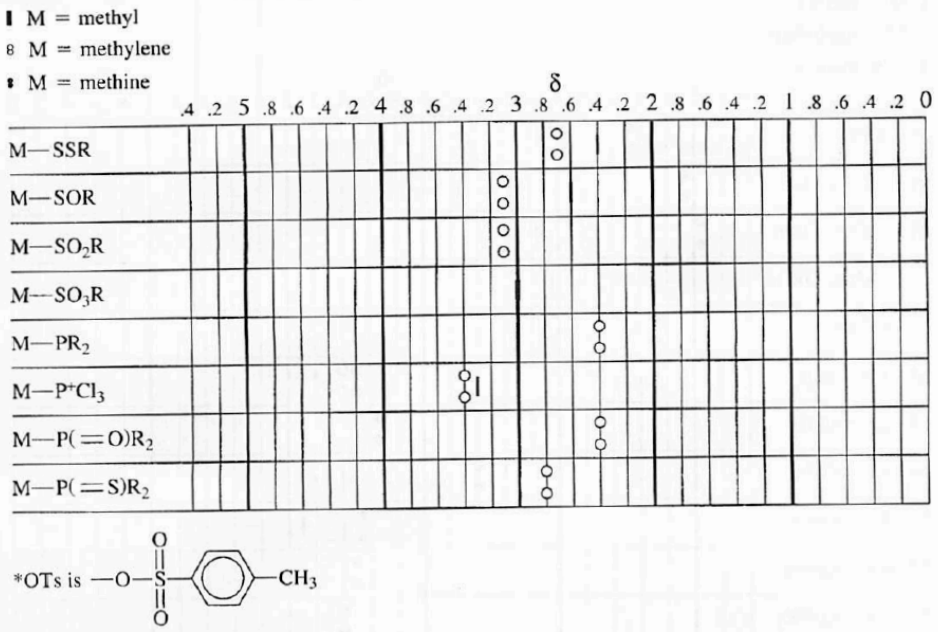


Table 13.1 (Continued)



*OTs is

Table 13.1 (Continued)

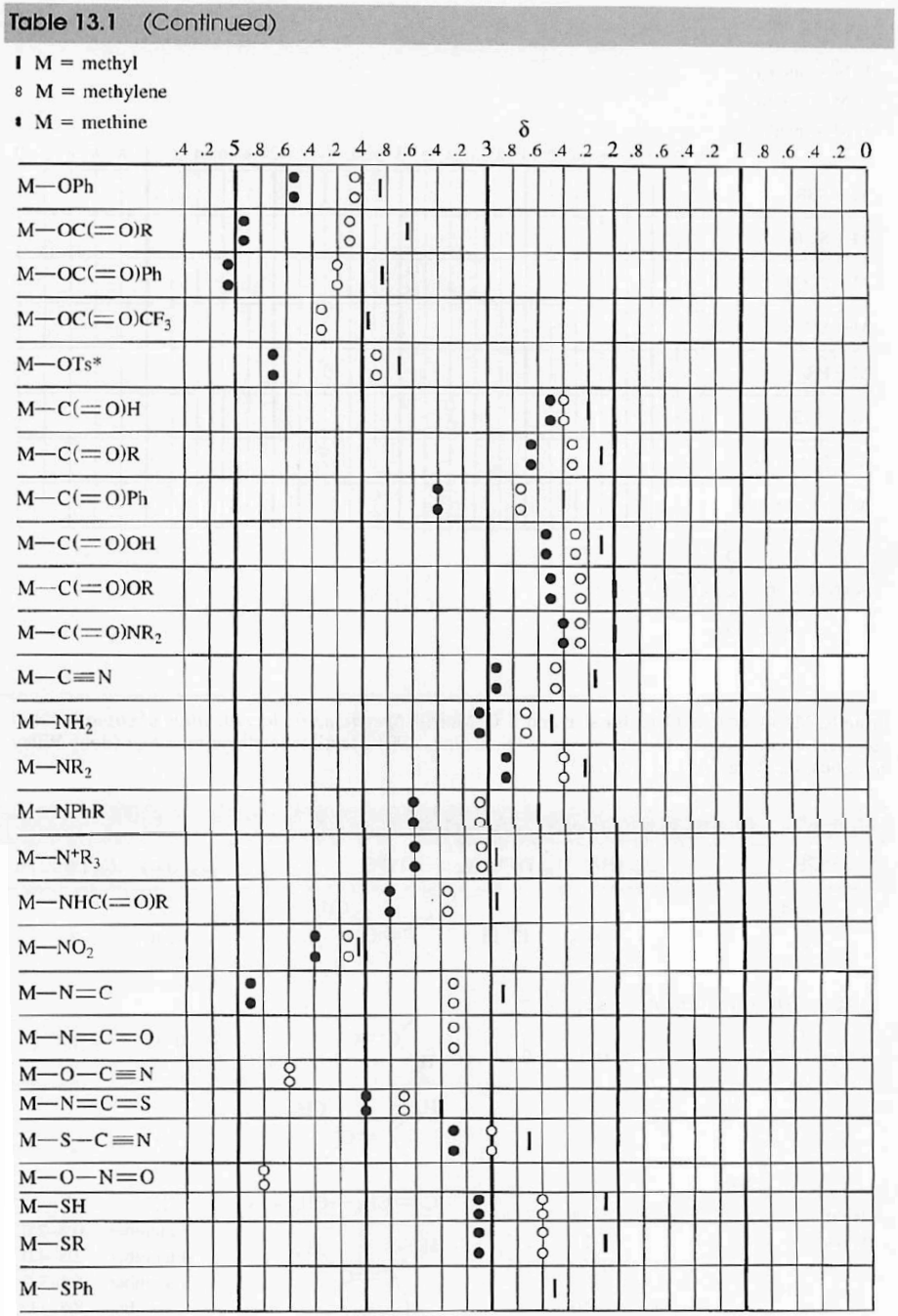
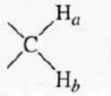
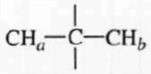
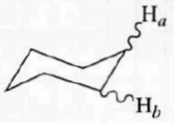
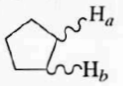


Table 13.2 Proton Spin-Coupling Constants

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	

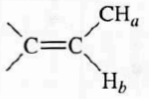
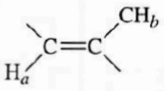
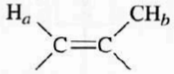
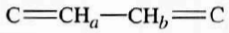
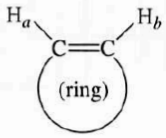
TYPE	J_{ab} (Hz)	J_{ab} TYPICAL
	4–10	7
	0–3	1.5
	0–3	2
	9–13	10
 (ring)	3 member 4 member 5 member 6 member 7 member 8 member	0.5–2.0 2.5–4.0 5.1–7.0 8.8–11.0 9–13 10–13

Table 13.3 Chemical Shifts in Alicyclic Rings

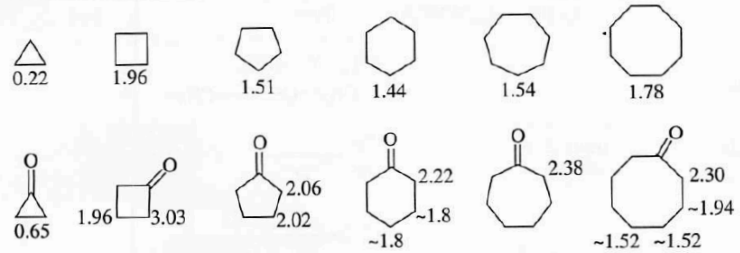
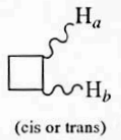
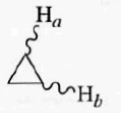
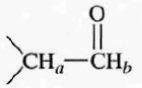
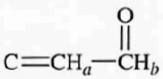
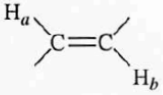
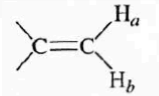
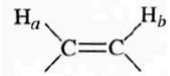
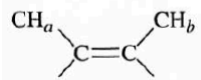
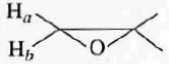
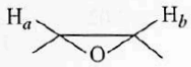
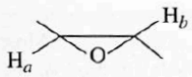
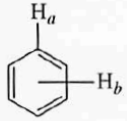
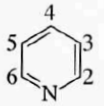
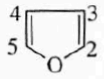
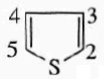


Table 14.3 Chemical Shifts of Alkyne Protons

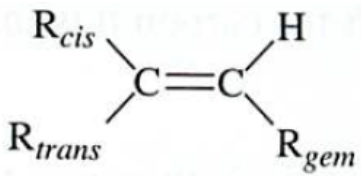
HC≡CR	1.73–1.88
HC≡C—COH	2.23
HC≡C—C≡CR	1.95
HC≡CH	1.80
HC≡CAR	2.71–3.37
HC≡C—C≡CR	2.60–3.10

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) *J* (meta) *J* (para)	6–10 1–3 0–1	9 3 ~0
	*J* (2–3) *J* (3–4) *J* (2–4) *J* (3–5) *J* (2–5) *J* (2–6)	(5–6) (7–9) (1–2) (1–2) (0–1) (0–1)	5 8 1.5 1.5 1 ~0
	*J* (2–3) *J* (3–4) *J* (2–4) *J* (2–5)	1.3–2.0 3.1–3.8 0–0 1–2	1..8 3.6 ~0 1.5
	*J* (2–3) *J* (3–4) *J* (2–4) *J* (2–5)	4.9–6.2 3.4–5.0 1.2–1.7 3.2–3.7	5.4 4.0 1.5 3.4

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

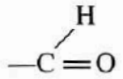
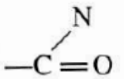
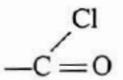
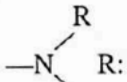
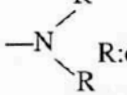


$$\delta_H = 5.25 + Z_{gem} + Z_{cis} + Z_{trans}$$

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