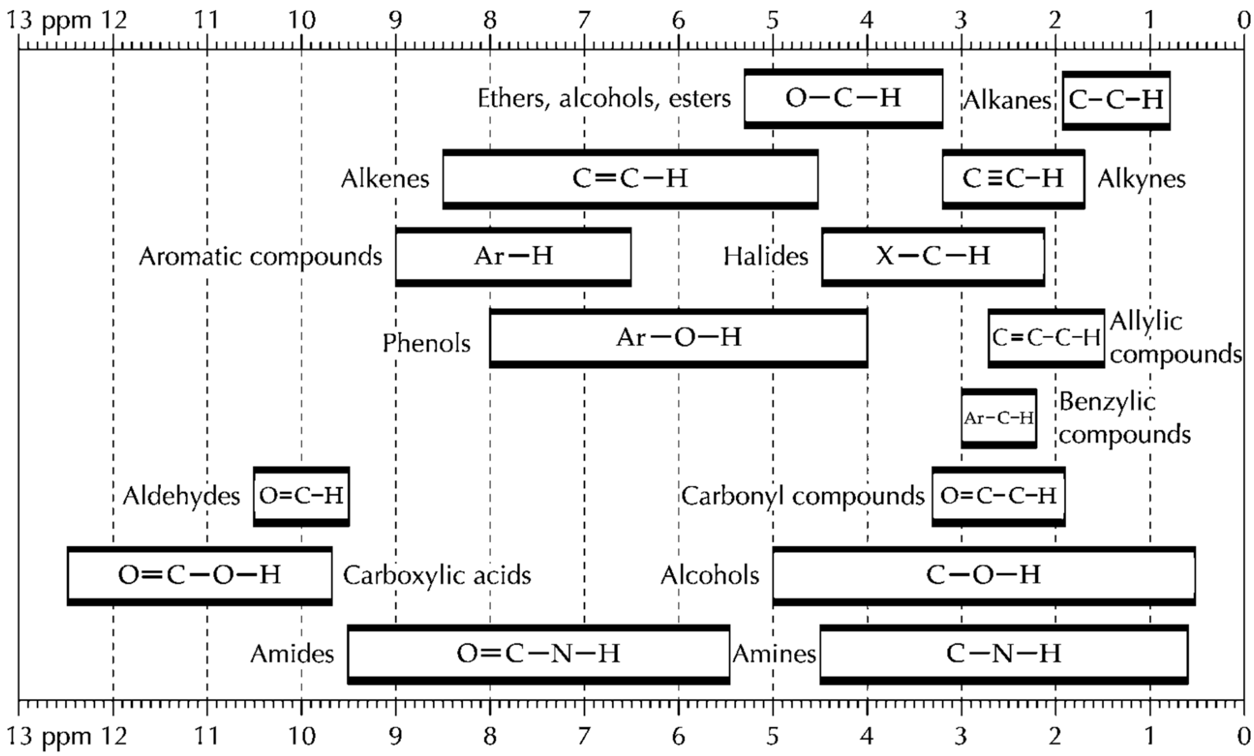

FIGURE 22.13 Approximate regions of chemical shifts for different types of protons in organic compounds.

TABLE 22.2 Characteristic ^{1}H NMR chemical shifts in $CDCl_3$

Compound	Chemical shift (δ, ppm)
TMS	0.0
Alkanes (C–C–**H**)	0.8–1.9
Amines (C–N–**H**)	0.6–4.5
Alcohols (C–O–**H**)	0.5–5.0
Alkenes[a] (C=C–C–**H**)	1.5–2.6
Alkynes (C≡C–**H**)	1.7–3.1
Carbonyl compounds (O=C–C–**H**)	1.9–3.3
Halides (X–C–**H**)	2.1–4.5
Aromatic compounds[b] (Ar–C–**H**)	2.2–3.0
Alcohols, esters, ethers (O–C–**H**)	3.2–5.3
Alkenes (C=C–**H**)	4.5–8.5
Phenols (Ar–O–**H**)	4.0–8.0
Amides (O=C–N–**H**)	5.5–9.5
Aromatic compounds (Ar–**H**)	6.5–9.0
Aldehydes (O=C–**H**)	9.5–10.5
Carboxylic acids (O=C–O–**H**)	9.7–12.5

a. Allylic protons.
b. Benzylic protons.

Figures from Mohrig's *Techniques in Organic Chemistry*, 3rd Edition.

TABLE 22.4 **Additive parameters for predicting NMR chemical shifts of aromatic protons in $CDCl_3$**

Base value 7.36 ppm[a]

Group	***ortho***	***meta***	***para***
—CH_3	–0.18	–0.11	–0.21
—$CH(CH_3)_2$	–0.14	–0.08	–0.20
—CH_2Cl	0.02	–0.01	–0.04
—CH=CH_2	0.04	–0.04	–0.12
—CH=CHAr	0.14	–0.02	–0.11
—CH=$CHCO_2H$	0.19	0.04	0.05
—CH=CH(C=O)Ar	0.28	0.06	0.05
Group	***ortho***	***meta***	***para***
—Ar	0.23	0.07	–0.02
—(C=O)H	0.53	0.18	0.28
—(C=O)R	0.60	0.10	0.20
—(C=O)Ar	0.45	0.12	0.23
—(C=O)CH=CHAr	0.67	0.14	0.21
—(C=O)OCH_3	0.68	0.08	0.19
—(C=O)OCH_2CH_3	0.69	0.06	0.17
—(C=O)OH	0.77	0.11	0.25
—(C=O)Cl	0.76	0.16	0.33
—(C=O)NH_2	0.46	0.09	0.17
—C≡N	0.29	0.12	0.25
—F	–0.32	–0.05	–0.25
—Cl	–0.02	–0.07	–0.13
—Br	0.13	–0.13	–0.08
—OH	–0.53	–0.14	–0.43
—OR	–0.45	–0.07	–0.41
—OAr	–0.36	–0.04	–0.28
—O(C=O)R	–0.27	0.02	–0.13
—O(C=O)Ar	–0.14	0.07	–0.09
—NH_2	–0.71	–0.22	–0.62
—$N(CH_3)_2$	–0.68	–0.15	–0.73
—NH(C=O)R	0.14	–0.07	–0.27
—NO_2	0.87	0.20	0.35

a. Base value is the measured chemical shift of benzene in $CDCl_3$ (1% solution).

TABLE 22.3 **Additive parameters for predicting NMR chemical shifts of alkyl protons in $CDCl_3$[a]**

Base values

Methyl	0.9 ppm
Methylene	1.2 ppm
Methine	1.5 ppm

Group (Y)	Alpha (α) substituent H—C—Y	Beta (β) substituent H—C—C—Y	Gamma (γ) substituent H—C—C—C—Y
—R	0.0	0.0	0.0
—C=C	0.8	0.2	0.1
—C=C–Ar[b]	0.9	0.1	0.0
—C=C(C=O)OR	1.0	0.3	0.1
—C≡C–R	0.9	0.3	0.1
—C≡C–Ar	1.2	0.4	0.2
—Ar	1.4	0.4	0.1
—(C=O)OH	1.1	0.3	0.1
—(C=O)OR	1.1	0.3	0.1
—(C=O)H	1.1	0.4	0.1
—(C=O)R	1.2	0.3	0.0
—(C=O)Ar	1.7	0.3	0.1
—(C=O)NH_2	1.0	0.3	0.1
—(C=O)Cl	1.8	0.4	0.1
—C≡N	1.1	0.4	0.2
—Br	2.1	0.7	0.2
—Cl	2.2	0.5	0.2
—OH	2.3	0.3	0.1
—OR	2.1	0.3	0.1
—OAr	2.8	0.5	0.3
—O(C=O)R	2.8	0.5	0.1
—O(C=O)Ar	3.1	0.5	0.2
—NH_2	1.5	0.2	0.1
—NH(C=O)R	2.1	0.3	0.1
—NH(C=O)Ar	2.3	0.4	0.1

a. There may be differences of 0.1–0.5 ppm in the chemical shift values calculated from this table and those measured from individual spectra.
b. Ar = aromatic group.

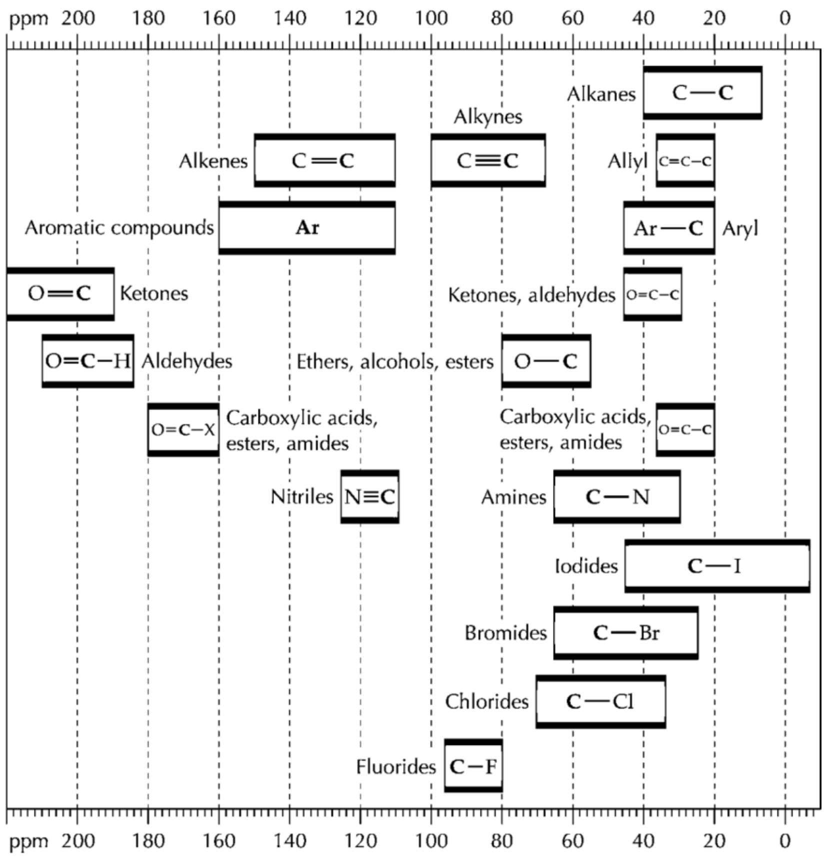

FIGURE 23.4 Approximate regions of ^{13}C chemical shifts for different types of carbon atoms in organic compounds.

TABLE 23.1 Characteristic ^{13}C NMR chemical shifts in $CDCl_3$

Compound	Chemical shift (ppm)
TMS	0.0
CDCl_3 (t)	77
Alkane (C–**C**H_3)	7–30
Alkane (C–**C**H_2)	15–40
Alkane (C–**C**H) and (C–**C**)	15–40
Carboxylic acids, esters, and amides (**C**–C=O)	20–35
Allyl (**C**–C=C)	20–35
Arene (**C**–Ar)	20–45
Ketones, aldehydes (**C**–C=O)	30–45
Amines (**C**–N)	30–65
Iodides (**C**–I)	–5–45
Bromides (**C**–Br)	25–65
Chlorides (**C**–Cl)	35–70
Fluorides (**C**–F)	80–95
Alcohols (**C**–OH), ethers (**C**–OR), esters (**C**–O[C=O]R)	55–80
Alkyne (**C**≡C)	70–100
Alkene (**C**=C)	110–150
Aromatic	110–160
Nitriles (**C**≡N)	110–125
Carboxylic acids, esters, and amides (**C**=O)	160–180
Aldehydes (**C**=O)	185–210
Ketones (**C**–O)	190–220

Figures from Mohrig’s *Techniques in Organic Chemistry*, 3rd Edition.