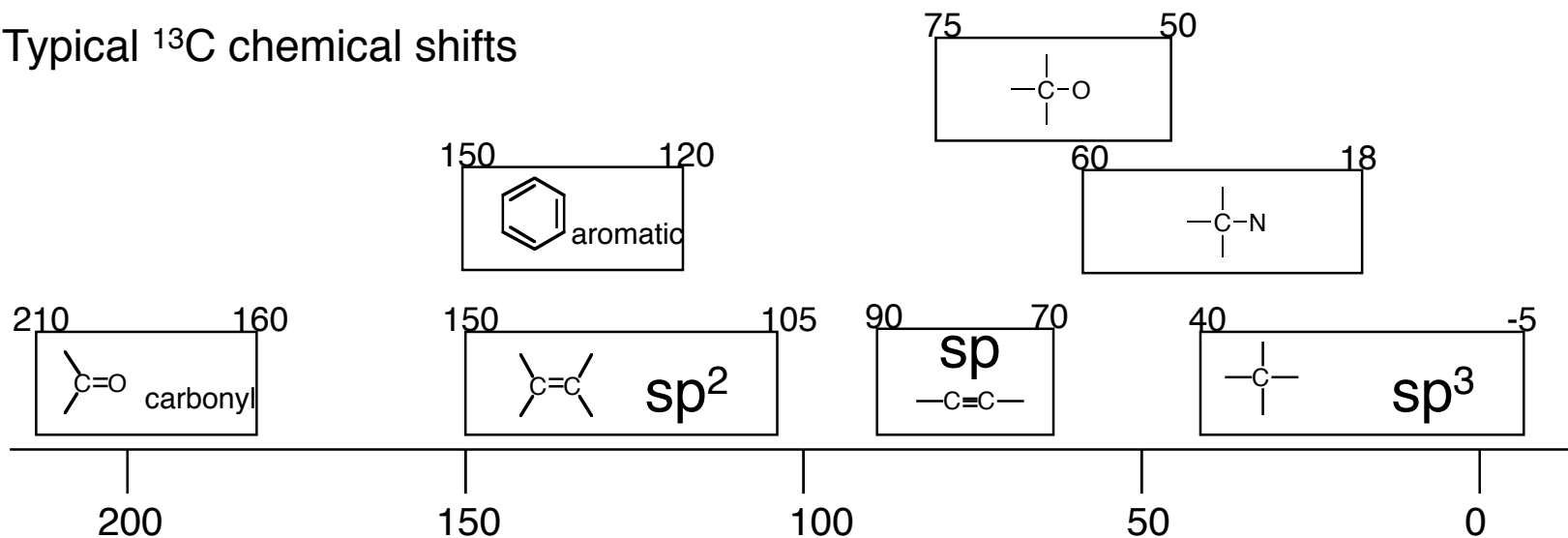


Carbon NMR essentials

You Should Know:

1. For $C_N H_{\#} O_{\#} N_{\#}$ $IHD = \frac{2N+2 - (\#hydrogens+\#halogens) + (\#Ns)}{2}$
2. How to identify symmetry and use it.
3. Proton Inventory. Identify if any protons are attached to non-carbon atoms by Summing the number of C-attached protons and comparing to molecular formula

4. Typical ^{13}C chemical shifts



5. multiplicities

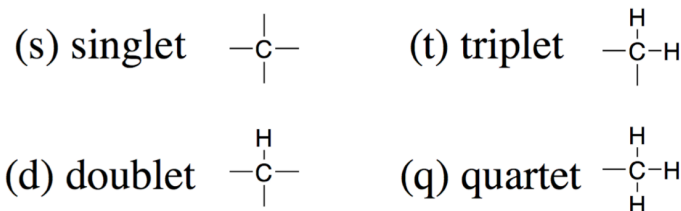
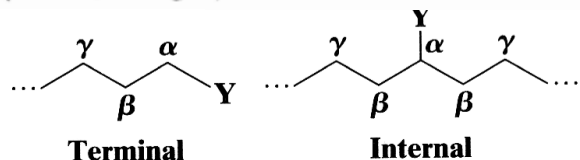
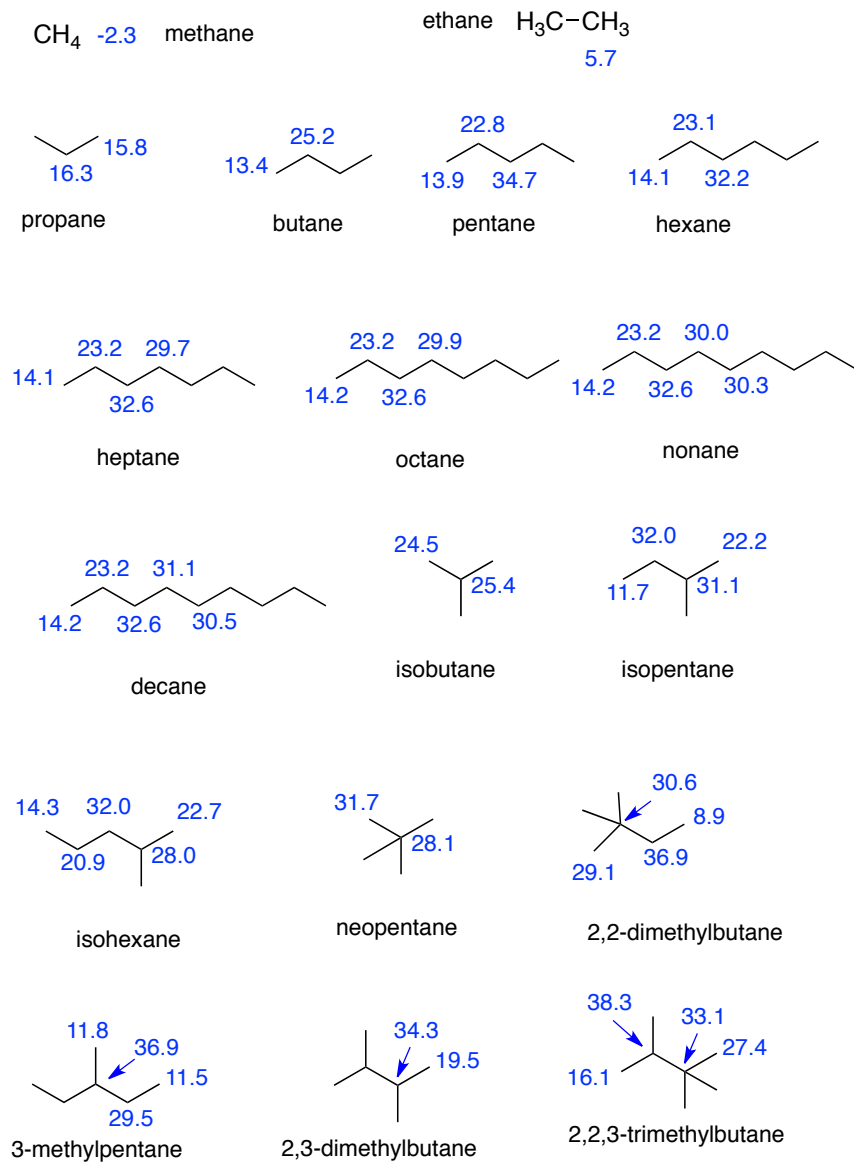


Table 5.3 Incremental Substituent Effects (ppm) on Replacement of H by Y in Alkanes. Y is Terminal or Internal^a (+ left, - right)

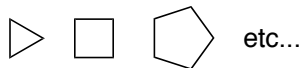


Y	Terminal		Internal		γ
	α	β	β	α	
CH ₃	+ 9	+ 6	+10	+ 8	-2
CH=CH ₂	+20		+ 6		-0.5
C≡CH	+ 4.5		+ 5.5		-3.5
COOH	+21	+16	+ 3	+ 2	-2
COO ⁻	+25	+20	+ 5	+ 3	-2
COOR	+20	+17	+ 3	+ 2	-2
COCl	+33	+28		+ 2	
CONH ₂	+22		+ 2.5		-0.5
COR	+30	+24	+ 1	+ 1	-2
CHO	+31		0		-2
Phenyl	+23	+17	+ 9	+ 7	-2
OH	+48	+41	+10	+ 8	-5
OR	+58	+51	+ 8	+ 5	-4
OCOR	+51	+45	+ 6	+ 5	-3
NH ₂	+29	+24	+11	+10	-5
NH ₃ ⁺	+26	+24	+ 8	+ 6	-5
NHR	+37	+31	+ 8	+ 6	-4
NR ₂	+42		+ 6		-3
NR ₃ ⁺	+31		+ 5		-7
NO ₂	+63	+57	+ 4	+ 4	
CN	+ 4	+ 1	+ 3	+ 3	-3
SH	+11	+11	+12	+11	-4
SR	+20		+ 7		-3
F	+68	+63	+ 9	+ 6	-4
Cl	+31	+32	+11	+10	-4
Br	+20	+25	+11	+10	-3
I	- 6	+ 4	+11	+12	-1

base values



Cycloalkanes



C_3H_6	-2.9	C_7H_{14}	28.4
C_4H_8	22.4	C_8H_{16}	26.9
C_5H_{10}	25.6	C_9H_{18}	26.1
C_6H_{12}	26.9	$C_{10}H_{20}$	25.3

Table 12.2 Saturated Heterocyclics

Unsubstituted

	39.5		18.7		18.2
	22.9		27.5		25.7
	26.5		31.2		27.8
	24.9		26.6		25.9
	27.7		27.8		27.8
	69.5		29.1		47.9
	68.4		31.7		47.1

Substituted

	47.6		24.4
	47.3		56.7
	18.1		48.0

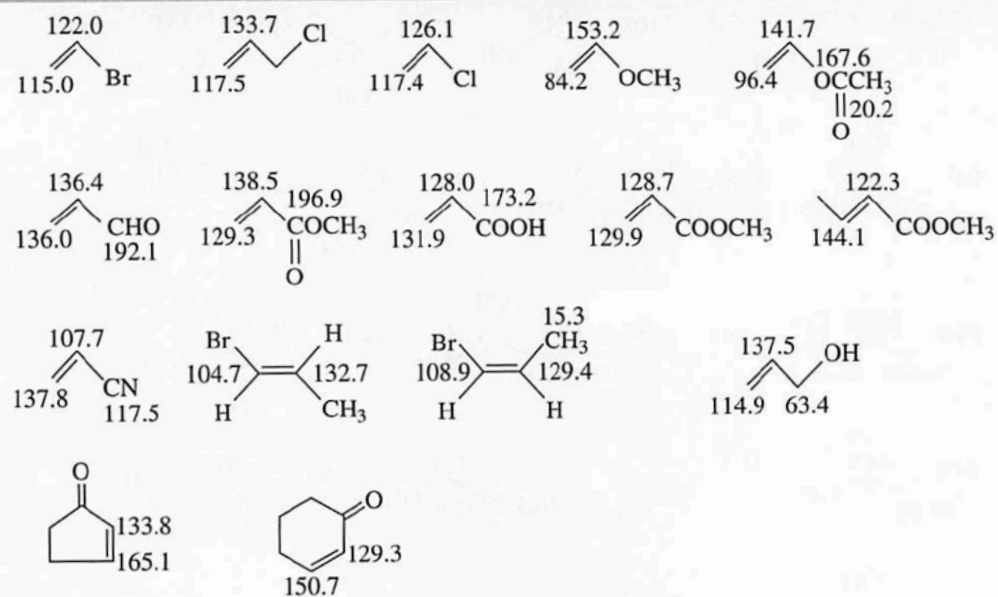
Table 12.3 Alkene and Cycloalkene Chemical Shifts (ppm from TMS)

$H_2C=CH_2$	123.2		136.2		113.3		12.1		126.0
	18.7		115.9		140.2		124.6		17.6
	114.3		14.0		132.7		123.2		138.7
	138.5		20.5		12.3		133.3		114.5
	13.7		35.3		125.1		131.2		13.7
	23.2		131.7		17.7		131.3		22.6
	117.5		115.9		114.4		129.5		18.0
	137.2		137.3		137.8		133.2		130.2
	109.3		16.9		116.5		130.9		12.8
	149.3		25.3		144.5		126.4		13.0
	131.4		118.7		112.9		131.6		128.3
	109.8		144.5		144.9		126.6		127.4
	30.2		137.2		107.1		149.7		26.0
	130.8		32.6		26.9		36.2		124.5
	22.1		22.1		28.9		26.9		22.3
	24.5		22.1		74.8		213.5		126.1
	22.1		22.1		124.6		124.6		22.3
	22.1		22.1		124.6		124.6		22.3

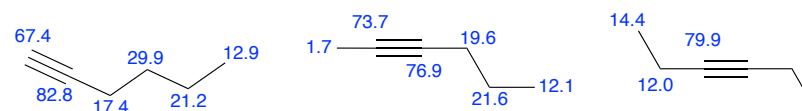
Alcohols

CH_3-OH	46.7	CH_3-CH_2-OH	27.3	$CH_3-C(OH)_2-CH_3$	32.0	$CH_3-C(OH)_2-CH_2-CH_3$	32.0
CH_3-CH_2-OH	64.9	$CH_3-CH_2-CH_2-OH$	25.2	$CH_3-C(OH)_2-CH_2-CH_3$	69.5	$CH_3-CH_2-CH_2-OH$	65.0
CH_3-CH_2-OH	18.1	$CH_3-CH_2-CH_2-OH$	10.1	$CH_3-CH_2-CH_2-OH$	19.2	$CH_3-CH_2-CH_2-OH$	19.2
CH_3-CH_2-OH	18.1	$CH_3-CH_2-CH_2-OH$	65.0	$CH_3-CH_2-CH_2-OH$	30.9	$CH_3-CH_2-CH_2-OH$	72.6

Table 12.4 Chemical Shifts of Substituted Alkenes (ppm from TMS)



Alkyne Chemical Shifts



Amine Chemical Shifts

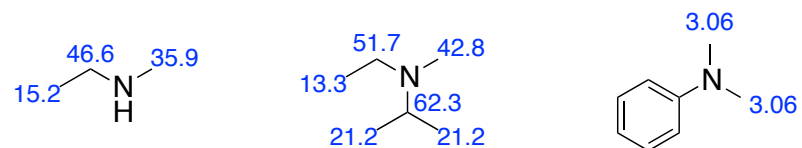
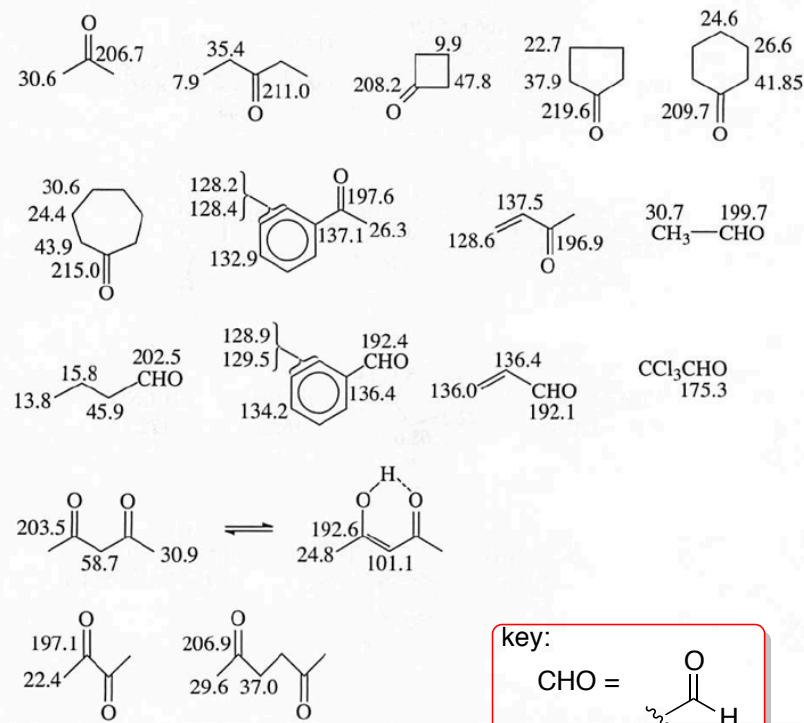


Table 12.8 Ketones and Aldehydes



key:
CHO =

Table 12.7 Chemical Shifts of Ethers, Acetals, and Epoxides

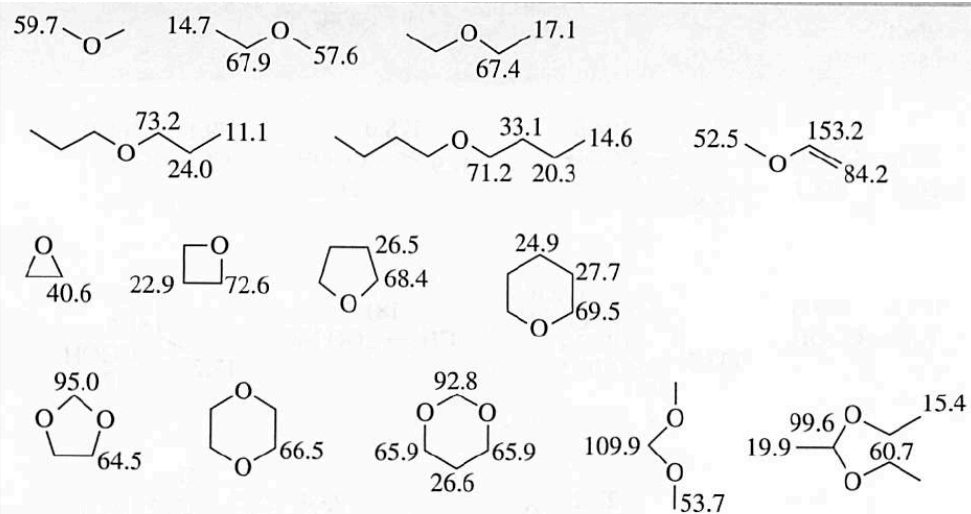
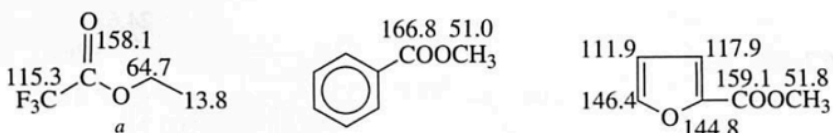
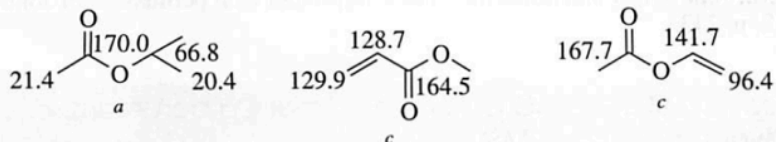
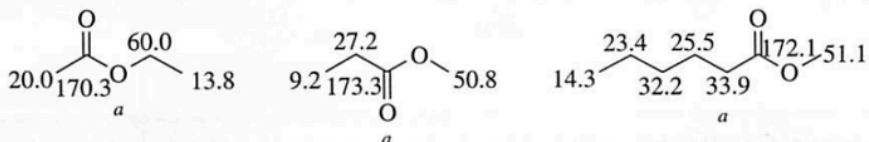
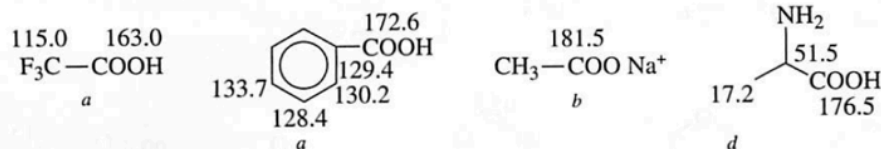
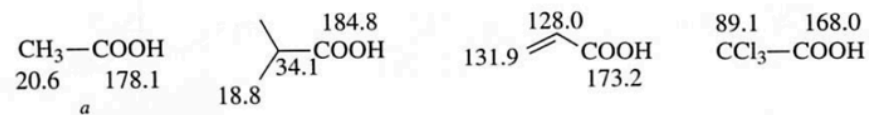


Table 12.9 Shift Positions for the C=O Group and Other Carbon Atoms of Carboxylic Acids, Esters, Lactones, Chlorides, Anhydrides, Amides, Carbamates, and Nitriles (ppm from TMS)



key:

