Carbon NMR essentials

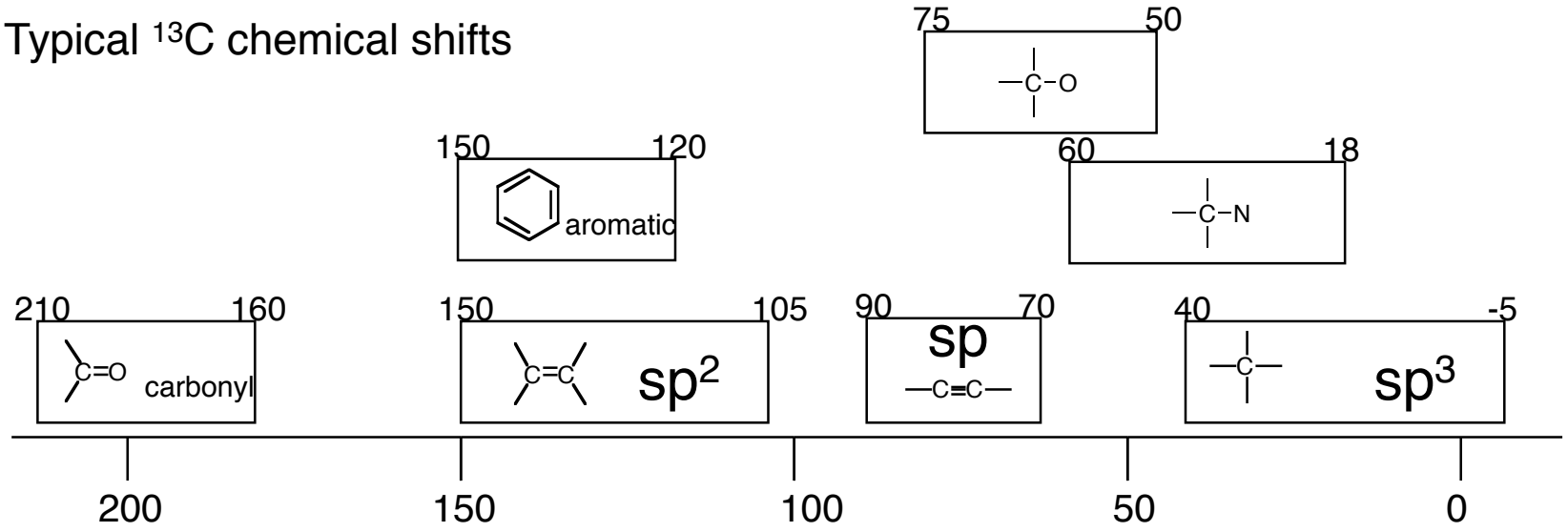
You Should Know:

1. For $C_NH_\#O_\#N_\#$ IHD = $\frac{2N+2 - (\#hydrogens+\#halogens) + (\#Ns)}{2}$

2. How to identify symmetry and use it.

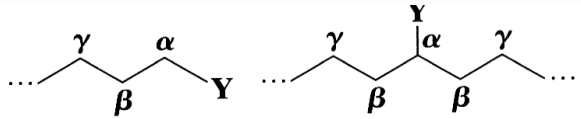
3. Proton Inventory. Identify if any protons are attached to non-carbon atoms by Summing the number of C-attached protons and comparing to molecular formula

4. Typical ^{13}C chemical shifts



5. multiplicities (s) singlet (t) triplet (d) doublet (q) quartet

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

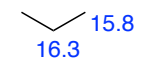


	α		β		γ
Y	**Terminal**	**Internal**	**Terminal**	**Internal**	
CH_3	+ 9	+ 6	+10	+ 8	−2
$CH{=}CH_2$	+20		+ 6		−0.5
$C{\equiv}CH$	+ 4.5		+ 5.5		−3.5
COOH	+21	+16	+ 3	+ 2	−2
COO^-	+25	+20	+ 5	+ 3	−2
COOR	+20	+17	+ 3	+ 2	−2
COCl	+33	+28		+ 2	
$CONH_2$	+22		+ 2.5		−0.5
COR	+30	+24	+ 1	+ 1	−2
CHO	+31		0		−2
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

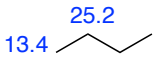
base values

CH_4 -2.3 methane

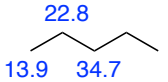
ethane $H_3C{-}CH_3$ 5.7



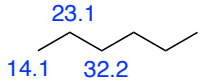
propane



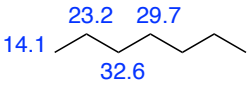
butane



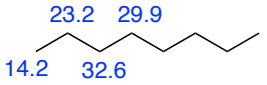
pentane



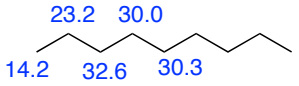
hexane



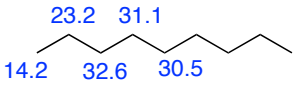
heptane



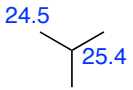
octane



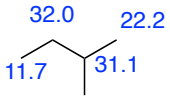
nonane



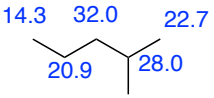
decane



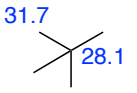
isobutane



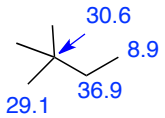
isopentane



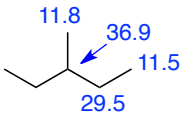
isohexane



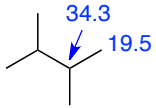
neopentane



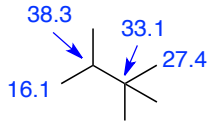
2,2-dimethylbutane



3-methylpentane

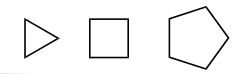


2,3-dimethylbutane



2,2,3-trimethylbutane

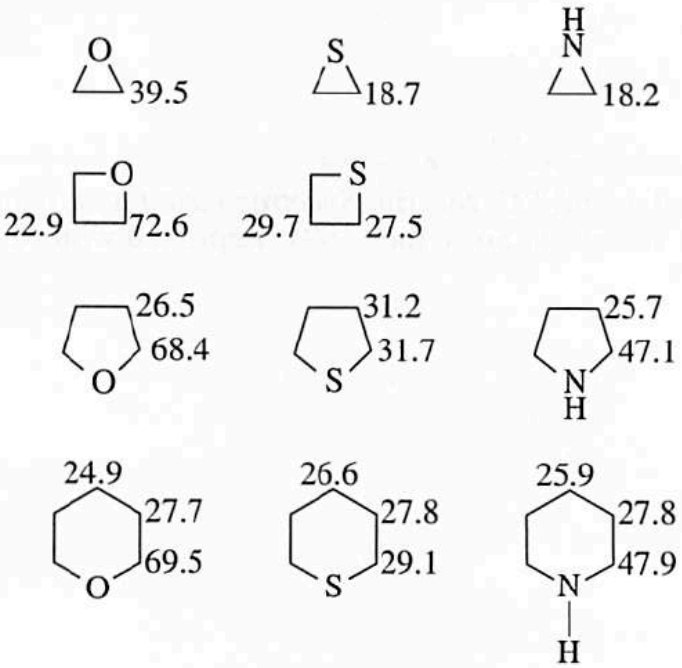
Cycloalkanes



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



Substituted

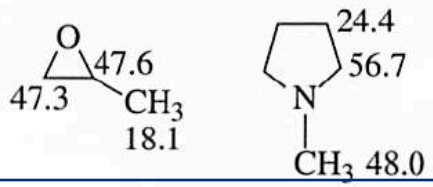
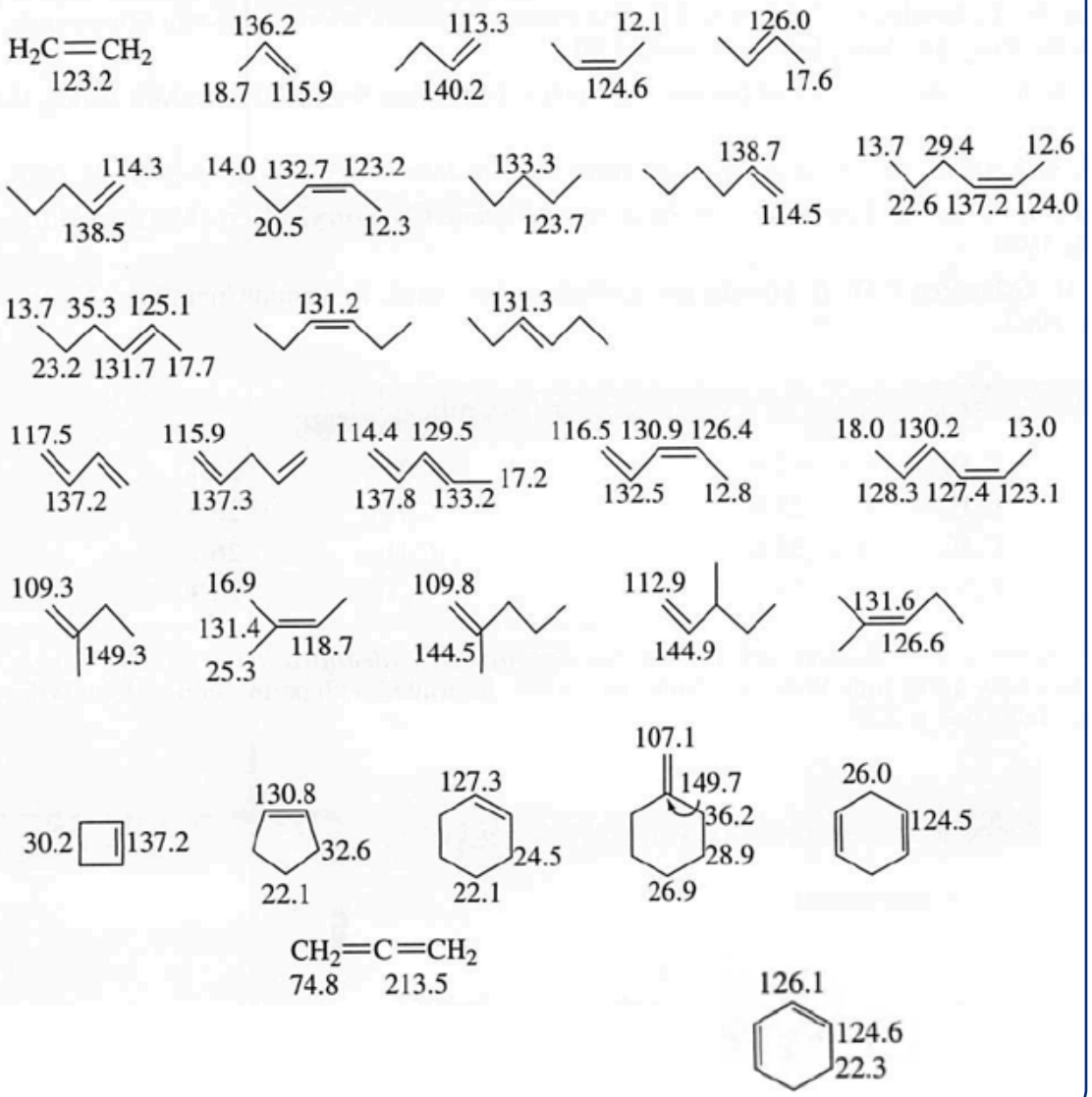


Table 12.3 Alkene and Cycloalkene Chemical Shifts (ppm from TMS)



Alcohols

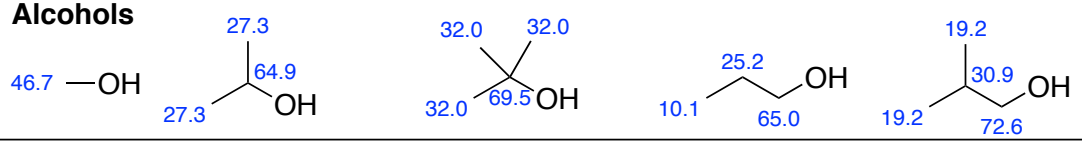


Table 12.4 Chemical Shifts of Substituted Alkenes (ppm from TMS)

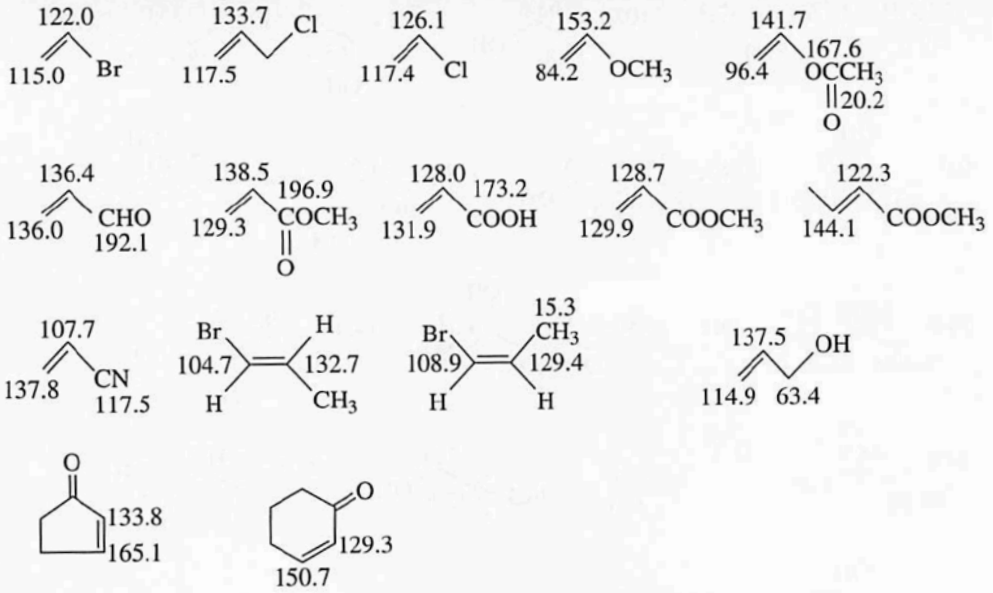
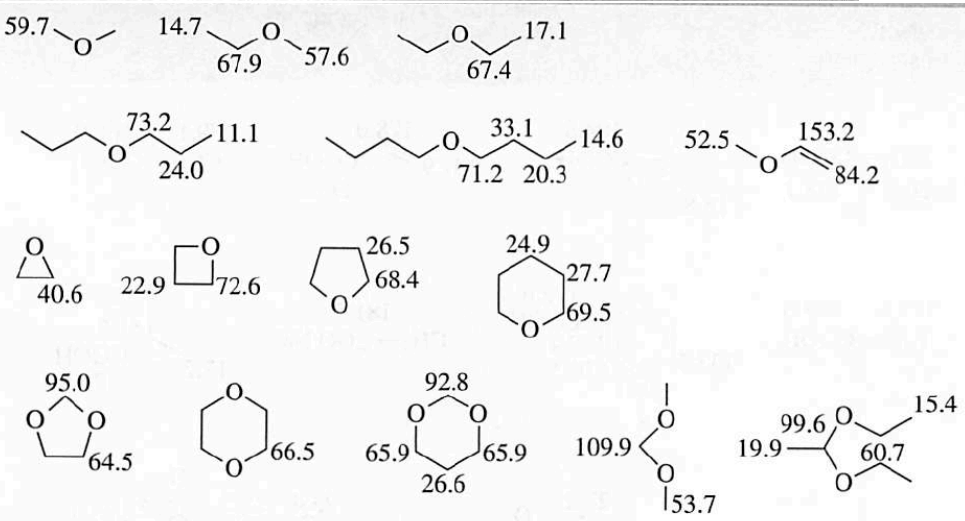
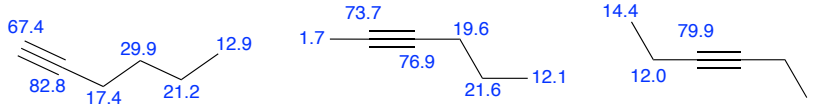


Table 12.7 Chemical Shifts of Ethers, Acetals, and Epoxides



Alkyne Chemical Shifts



Amine Chemical Shifts

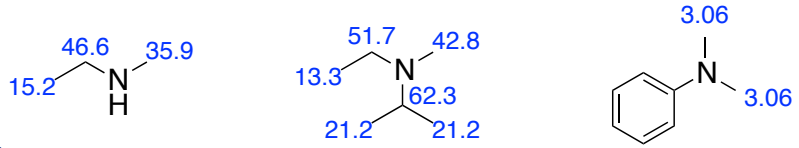


Table 12.8 Ketones and Aldehydes

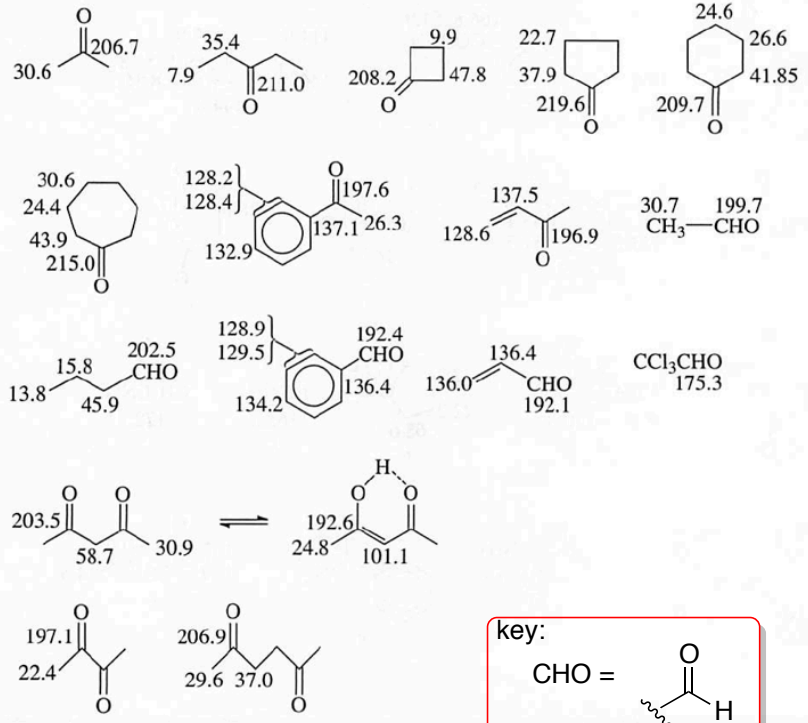


Table 12.9 Shift Positions for the C=O Group and Other Carbon Atoms of Carboxylic Acids, Esters, Lactones, Chlorides, Anhydrides, Amides, Carbamates, and Nitriles (ppm from TMS)