
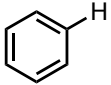


Organic Spectroscopy Values

Quick Reference (*all numbers approximate*)

^1H NMR chemical shifts (ppm)

$\begin{array}{c} \text{---} \\ \\ \text{H}-\text{C}-\text{SiR}_3 \\ \\ \text{---} \end{array}$	0		0.5	
$\begin{array}{c} \text{---} \\ \\ \text{H}-\text{C}-\text{CR}_3 \\ \\ \text{---} \end{array}$	1	$\equiv\text{C}-\text{H}$	3	
$\begin{array}{c} \text{---} \\ \\ \text{H}-\text{C}-\text{NR}_2 \\ \\ \text{---} \end{array}$	2	$\text{C}=\text{C}-\text{H}$	5-6	} 1.5-3 allylic α -carbonyl benzylic
$\begin{array}{c} \text{---} \\ \\ \text{H}-\text{C}-\text{OR} \\ \\ \text{---} \end{array}$	3		7.5	
$\begin{array}{c} \text{---} \\ \\ \text{H}-\text{C}-\text{F} \\ \\ \text{---} \end{array}$	4	$\text{C}=\text{O}-\text{H}$	9	

Protons exchanging with D_2O as a sign of acidity:

OH δ 2 – 20 ppm NH δ 4–8 (usually singlet)

Negative δ :

Metal hydrides or protons “inside” an aromatic system e.g. annulenes

Multiplicity and J values (Hz):

3H, singlet $\text{>C}-\text{CH}_3$ 3H, doublet $\text{H}-\text{C}-\text{CH}_3$

3H, triplet + 2H, quartet (identical J value) CH_2CH_3

5H, broad singlet (δ approx. 7 ppm) Ph

2 x 1H, doublet (J approx. 7 Hz)



2 x 1H, doublet (J approx. 12 Hz)



3 x 1H, doublet of doublets (3 different J values)



Infra-red Spectra (cm^{-1})

3700-2700	2300-1900	1850-1600	1600-600	cm^{-1}
X-H	X \equiv Y X=Y=Z	X=Y	X-Y bending stretching	

3700-2700 cm^{-1} region:

C-H - 3000

Aldehyde C-H - 2750

O-H - 3000-3600

N-H - 3300-3500

H-bonding broadens and shifts to lower frequency.

1850-1600 cm^{-1} region:

Ketone C=O - 1715

Aldehyde C=O - 1730

Ester C=O - 1745

Acid C=O - 1700 (depends on extent of H-bonding)

Amide C=O - 1650

Imine C=N - 1650

Conjugation lowers the stretching frequency by approx. 30cm^{-1}

Ring strain increases the stretching frequency by approx. 30cm^{-1} for progressively smaller ring sizes.

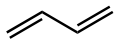
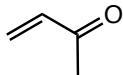
C=C - 1640 weak (possibly not seen) unless conjugated with e.g. C=O

Ultra Violet Spectra (nm)

Forbidden (weak) bands: ϵ 10-100:

$n \rightarrow \pi^*$	$C=C$	160 nm
	$C=O$	285 nm
$n \rightarrow \sigma^*$	$C-OR$	190 nm
	$C-NR_2$	230 nm

Allowed (intense) bands: $\epsilon > 10,000$:

$\pi \rightarrow \pi^*$		217 nm	to longer λ if conjugated: +60 nm for $C=C$ or Ar +5-10 nm for alkyl C groups +0-50 nm for lone pairs
		225 nm	
<i>cis</i> shorter λ lower ϵ	<i>trans</i> longer λ higher ϵ	also applies to s-cis vs. s-trans	

Aromatics:

e.g. benzene 180nm (ϵ 60,000), 200nm (ϵ 7,000), 250nm (ϵ 200)

Conjugation and substitution both shift to longer wavelength

Spectra of phenols and amines change with pH.