

## **<sup>1</sup>H Nuclear Magnetic Resonance Chemical Shifts**

Chemical Shifts in ppm downfield from tetramethylsilane (defined as  $\delta = 0.000$  ppm). Values are approx.  $\pm 0.2$  ppm).

### **Protons on a Carbon Adjacent to a Functional Group**

Functional Group	<u>CH<sub>3</sub></u>		<u>CH<sub>2</sub></u>		<u>CH</u>	
	$\delta$	( $\Delta\delta$ )	$\delta$	( $\Delta\delta$ )	$\delta$	( $\Delta\delta$ )
saturated system	0.8		1.2		1.6	
M-C=C	1.6	(0.8)	2.0	(0.8)	2.4	(0.8)
M-C $\equiv$ C	1.7	(0.9)	2.2	(1.0)	2.8	(1.2)
M-Phenyl	2.2	(1.4)	2.6	(1.4)	2.8	(1.2)
M-Cl	3.0	(2.2)	3.4	(2.2)	4.0	(2.4)
M-Br	2.7	(1.9)	3.4	(2.2)	4.1	(2.5)
M-I	2.2	(1.4)	3.1	(1.9)	4.2	(2.6)
M-OH	3.2	(2.4)	3.4	(2.2)	3.8	(2.2)
M-OR	3.2	(2.4)	3.4	(2.2)	3.6	(2.0)
M-O-Phenyl	3.9	(3.1)	4.1	(2.9)	4.5	(2.9)
M-OC(=O)R	3.6	(2.8)	4.1	(2.9)	4.5	(2.9)
M-OC(=O)Ph	3.8	(3.0)	4.2	(3.0)	5.0	(3.4)
M-CH=O (aldehyde)	2.2	(1.4)	2.4	(1.2)	2.5	(0.9)
M-C(R)=O (ketone)	2.1	(1.3)	2.3	(1.1)	2.6	(1.0)
M-COOH (acid)	2.1	(1.3)	2.3	(1.1)	2.5	(0.9)
M-COOR (ester)	2.0	(1.2)	2.2	(1.0)	2.5	(0.9)
M-NR <sub>2</sub>	2.4	(1.6)	2.6	(1.4)	2.9	(1.3)
M-NHC(=O)R	2.9	(2.1)	3.3	(2.1)	3.9	(2.3)

### **Protons on a Carbon Once Removed from a Functional Group**

Functional Group	<u>CH<sub>3</sub></u>		<u>CH<sub>2</sub></u>		<u>CH</u>	
	$\delta$	( $\Delta\delta$ )	$\delta$	( $\Delta\delta$ )	$\delta$	( $\Delta\delta$ )
M-C-CH <sub>2</sub>	0.8		1.2		1.6	
M-C-C=C	1.0	(0.2)	1.55	(0.35)	1.8	(0.2)
M-C-C $\equiv$ C	1.2	(0.4)	1.5	(0.3)	1.8	(0.2)
M-C-Ph	1.2	(0.4)	1.6	(0.4)	1.8	(0.2)
M-C-Cl	1.5	(0.7)	1.8	(0.6)	2.0	(0.4)
M-C-Br	1.8	(1.0)	1.9	(0.7)	1.9	(0.3)
M-C-I	1.8	(1.0)	1.8	(0.6)	2.1	(0.5)
M-C-OH (or OR)	1.2	(0.4)	1.5	(0.3)	1.8	(0.2)
M-C-OPh	1.3	(0.5)	1.6	(0.4)	2.0	(0.4)
M-C-OC(=O)R	1.3	(0.5)	1.6	(0.4)	1.8	(0.2)
M-C-CH=O	1.1	(0.3)	1.6	(0.4)	2.0	(0.4)
M-C-C(R)=O	1.1	(0.3)	1.6	(0.4)	2.0	(0.4)
M-C-CO <sub>2</sub> R	1.1	(0.3)	1.7	(0.5)	1.9	(0.3)
M-C-NR <sub>2</sub>	1.0	(0.2)	1.5	(0.3)	1.7	(0.1)
M-C-NH-C(=O)R	1.1	(0.3)	1.5	(0.3)	1.9	(0.3)

### Protons on $sp^2$ and $sp$ Hybridized Carbons

$R_2C=CH_2$	4.7-5.3	$C=CH-C=O$	6.0
$R_2C=CHR$	5.1	$C=CH-Cl$	6.5
$RCH=CHR$	5.3	$C=CHBr$	6.5
cyclohexene	5.6	$CH=CH-C=O$	6.9
$ArCH=C-C=O$	7.7	$RCH=O$	9.1
$R-C\equiv C-H$	2.3-3.3	R-OH (alcohol)	0.5-5.5
Aromatic hydrogens	6.0-9.0 (mostly 6.7-8.2)	R-NHR (amine)	0.5-5.0
$R-C(=O)OH$	12-14	R-NH-C(=O)R (amide)	5-8

### Nuclear Magnetic Resonance Chemical Shifts

Chemical Shifts in ppm downfield from tetramethylsilane (TMS) (defined as  $\delta = 0.000$  ppm).

General Regions:

0 - 1 $\delta$	cyclopropyl hydrogens and methyl groups not shifted by electronegative atoms
1 - 2 $\delta$	methyl groups $\beta$ - to O or N atoms, attached to C=C or attached to aromatic rings; methylene groups
2 - 3 $\delta$	methyl and methylene groups next to carbonyls or attached directly to nitrogen of amines
3 - 4 $\delta$	methyl and methylene groups attached to oxygen or halogens (Br, Cl). $C=CH_2$ groups
4.5 - 6.5 $\delta$	hydrogens on $sp^2$ hybridized carbons of alkenes (not aromatics)
6.8 - 8.5 $\delta$	aromatic protons
9 - 10 $\delta$	<u>aldehyde protons</u>

**IMPORTANT AND DIAGNOSTIC INFRARED BANDS**  
(a very condensed table)

<u><math>\nu</math> (cm<sup>-1</sup>)</u>		<u>Comments</u>
3000-3400	O-H stretching	alcohols- unassociated OH's - 2 bands around 3600 (sharp) H-bonded - broad absorption at 3400 acids- very broad, centred at ca. 3000
3400-3200	N-H stretching	amines- unassociated NH's - 2 bands around 3400 (sharp) H-bonded - broad absorption at 3200, weaker than OH
3300	C-H stretching of an acetylene	
3100-2850	C-H stretching	sp <sup>2</sup> - hybridized > 3000; sp <sup>3</sup> - hybridized < 3000
2900-2700	C-H stretching of ALDEHYDE	
2250-2100	C≡C stretching of ALKYNE	usually weak (weaker than C≡N), unless conjugated to C=O
2250-2225	C≡N stretching of NITRILE	2250 if not conjugated, 2225 conjugated Band <u>may</u> be weak
1800	C=O stretching of ACID CHLORIDE	>>>>
		>>>>
		>>>>
1735-1740	C=O stretching of ESTER	>>>>
		>>>>
		>>>>
1730	C=O stretching of ALDEHYDE	>>>>
		>>>>
		>>>>
1710	C=O stretching of KETONE	>>>>
		>>>>
		>>>>
1700	C=O stretching of ACID	>>>>
		>>>>
		>>>>
1660	C=O stretching of AMIDE	>>>>
		>>>>
		>>>>
1650-1600	C=C stretch	may be weak. Intensity increases with conjugation, especially to C=O

**Conjugation LOWERS these**

**bands by 30 cm<sup>-1</sup>**

**Being in a 5-membered ring**

**raises these bands by 35 cm<sup>-1</sup>**