

**NMR Spectroscopy****SOME POINTS TO REMEMBER****Table:** Frequencies and Field Strengths at which selected nuclei have their nuclear resonances

Isotope	Natural Abundance (%)	Field Strength, B_0 (Tesla)	Frequency, ν (MHz)	Magnetogyric Ratio, γ (10^6 radians/Tesla \times sec.)
^1H	99.98	1.00	42.6	267.53
		1.41	60.0	
		2.35	100.0	
		4.70	200.0	
		7.05	300.0	
^2H	0.0156	1.00	6.5	41.1
^{13}C	1.108	1.00	10.7	67.28
		1.41	15.1	
		2.35	25.0	
		4.70	50.0	
		7.05	75.0	
^{19}F	100.0	1.00	40.0	251.7
^{31}P	100.0	1.00	17.2	108.3

Table: Approximate Chemical Shift Ranges (PPM) for Selected Types of Protons

$\text{R}-\text{CH}_3$	0.7 – 1.3	$\text{R}-\text{CH}_2-\text{R}$	1.2 – 1.4
R_3CH	1.4 – 1.7	$\text{R}-\overset{\text{H}}{\underset{\text{H}}{\text{C}}}=\overset{\text{H}}{\underset{\text{H}}{\text{C}}}-\overset{\text{H}}{\underset{\text{H}}{\text{C}}}-\text{H}$	1.6 – 2.6
$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\overset{\text{H}}{\underset{\text{H}}{\text{C}}}-\text{H}; \text{H}-\overset{\text{O}}{\parallel}{\text{C}}-\overset{\text{H}}{\underset{\text{H}}{\text{C}}}-\text{H}$	2.1 – 2.4	$\text{RO}-\overset{\text{O}}{\parallel}{\text{C}}-\overset{\text{H}}{\underset{\text{H}}{\text{C}}}-\text{H}; \text{H}-\overset{\text{O}}{\parallel}{\text{C}}-\overset{\text{H}}{\underset{\text{H}}{\text{C}}}-\text{H}$	2.1 – 2.5

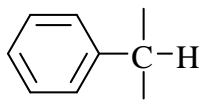
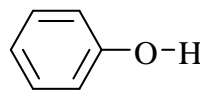
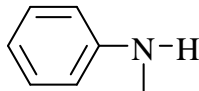
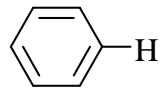
$\text{N} \equiv \text{C} - \underset{\text{ }}{\overset{\text{ }}{\text{C}}} - \text{H}$	2.1 – 3.0		2.3 – 2.7
$\text{R} - \text{C} \equiv \text{C} - \text{H}$	1.7 – 2.7	$\text{R} - \text{S} - \text{H}$	var 1.0 – 4.0
$\text{R} - \underset{\text{ }}{\text{N}} - \text{H}$	var 0.5 – 4.0	$\text{R} - \text{O} - \text{H}$	var 0.5 – 5.0
	var 4.0 – 7.0		var 3.0 – 5.0
$\text{R} - \overset{\text{O}}{\parallel} \text{C} - \underset{\text{ }}{\text{N}} - \text{H}$	var 5.0 – 9.0	$\text{R} - \underset{\text{ }}{\text{N}} - \underset{\text{ }}{\text{C}} - \text{H}$	2.2 – 2.9
$\text{R} - \text{S} - \underset{\text{ }}{\text{C}} - \text{H}$	2.0 – 3.0	$\text{I} - \underset{\text{ }}{\text{C}} - \text{H}$	2.0 – 4.0
$\text{Br} - \underset{\text{ }}{\text{C}} - \text{H}$	2.7 – 4.1	$\text{Cl} - \underset{\text{ }}{\text{C}} - \text{H}$	3.1 – 4.1
$\text{R} - \overset{\text{O}}{\parallel} \text{S} - \text{O} - \underset{\text{ }}{\text{C}} - \text{H}$	3.0	$\text{RO} - \underset{\text{ }}{\text{C}} - \text{H}, \text{OH} - \underset{\text{ }}{\text{C}} - \text{H}$	3.2 – 3.8
$\text{R} - \overset{\text{O}}{\parallel} \text{C} - \text{O} - \underset{\text{ }}{\text{C}} - \text{H}$	3.5 – 4.8	$\text{O}_2\text{N} - \underset{\text{ }}{\text{C}} - \text{H}$	4.1 – 4.3
$\text{F} - \underset{\text{ }}{\text{C}} - \text{H}$	4.2 – 4.8	$\text{R} - \underset{\text{ }}{\text{C}} = \underset{\text{ }}{\text{C}} - \text{H}$	4.5 – 6.5
	6.5 – 8.0	$\text{R} - \overset{\text{O}}{\parallel} \text{C} - \text{H}$	9.0 – 10.0
$\text{R} - \overset{\text{O}}{\parallel} \text{C} - \text{OH}$	11.0 – 12.0		

Table: Typical Ranges For Protons With Variable Chemical Shift

Acids	RCOOH	10.5 – 12.0 ppm
Phenols	ArOH	4.0 – 7.0
Alcohols	ROH	0.5 – 5.0
Amines	RNH_2	0.5 – 5.0
Amides	RCONH_2	5.0 – 8.0
Enols	$\text{CH}=\text{CH}-\text{OH}$	> 15

Table: Some Commonly Observed Splitting Patterns














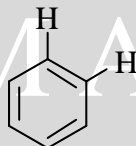
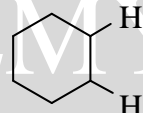
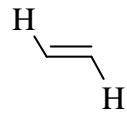
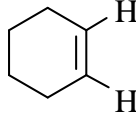
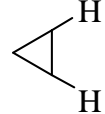
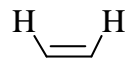
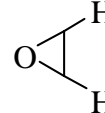
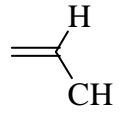
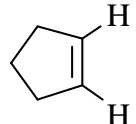
	$\begin{array}{c} \quad \\ \text{X}-\text{CH}-\text{CH}-\text{Y} \\ (\text{X} \neq \text{Y}) \end{array}$	
	$\begin{array}{c} \\ -\text{CH}_2-\text{CH} \\ \end{array}$	
	$\begin{array}{c} \text{X}-\text{CH}_2-\text{CH}_2-\text{Y} \\ (\text{X} \neq \text{Y}) \end{array}$	
	$\begin{array}{c} \\ \text{CH}_3-\text{CH} \\ \end{array}$	
	CH_3-CH_2-	
	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH} \\ \\ \text{CH}_3 \end{array}$	

Table: Some Representative Coupling Constants and Their approximate values (HZ)

	6 to 8		ortho 6 to 10		a, a 8 to 14 a, e 0 to 7 e, e 0 to 5
	11 to 18		8 to 11		cis 6 to 12 trans 4 to 8
	6 to 15				cis 2 to 5 trans 1 to 3
	4 to 10				5 to 7