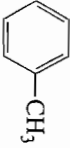
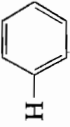


**Table 13.1** Approximate Values of Chemical Shifts for  $^1\text{H}$  NMR<sup>a</sup>

Type of proton	Approximate chemical shift (ppm)	Type of proton	Approximate chemical shift (ppm)
$-\text{CH}_3$	0.85	$\text{I}-\text{C}-\text{H}$	2.5-4
$-\text{CH}_2-$	1.20		
$-\text{CH}-$	1.55	$\text{Br}-\text{C}-\text{H}$	2.5-4
$-\text{C}=\text{C}-\text{CH}_3$	1.7	$\text{Cl}-\text{C}-\text{H}$	3-4
$-\text{C}-\text{CH}_3$	2.1	$\text{F}-\text{C}-\text{H}$	4-4.5
	2.3	$\text{RNH}_2$	Variable,
$-\text{C}\equiv\text{C}-\text{H}$	2.4	$\text{ROH}$	Variable,
$\text{R}-\text{O}-\text{CH}_3$	3.3	$\text{ArOH}$	Variable,
$\text{R}-\text{C}=\text{CH}_2$	4.7		6.5-8
$\text{R}-\text{C}=\text{C}-\text{H}$	5.3	$\text{C}=\text{O}-\text{H}$	9.0-10
		$\text{C}=\text{O}-\text{OH}$	Variable
		$\text{C}=\text{O}-\text{NH}_2$	Variable

<sup>a</sup>The values are approximate because they are affected by neighboring substituents.

**Table IR.1** A Simplified Correlation Table

Type of Vibration	Frequency ( $\text{cm}^{-1}$ )	Intensity
$\text{C}-\text{H}$ Alkanes (stretch)	3000-2850	s
$-\text{CH}_3$ (bend)	1450 and 1375	m
$-\text{CH}_2-$ (bend)	1465	m
Alkenes (stretch)	3100-3000	m
(bend)	1700-1000	s
Aromatics (stretch)	3150-3050	s
(out-of-plane bend)	1000-700	s
Alkyne (stretch)	ca. 3300	s
Aldehyde	2900-2800	w
	2800-2700	w
$\text{C}-\text{C}$ Alkane	Not interpretatively useful	
$\text{C}=\text{C}$ Alkene	1680-1600	m-w
Aromatic	1600-1400	m-w
$\text{C}\equiv\text{C}$ Alkyne	2250-2100	m-w
$\text{C}=\text{O}$ Aldehyde	1740-1720	s
Ketone (acyclic)	1725-1705	s
Carboxylic acid	1725-1700	s
Ester	1750-1730	s
Amide	1700-1640	s
Anhydride	ca. 1810	s
	ca. 1760	s
$\text{C}-\text{O}$ Alcohols, ethers, esters, carboxylic acids	1300-1000	s
$\text{O}-\text{H}$ Alcohol, phenols		
Free	3650-3600	m
H-Bonded	3400-3200	m
Carboxylic acids	3300-2500	m
$\text{N}-\text{H}$ Primary and secondary amines	ca. 3500	m
$\text{C}\equiv\text{N}$ Nitriles	2260-2240	m
$\text{N}=\text{O}$ Nitro ( $\text{R}-\text{NO}_2$ )	1600-1500	s
	1400-1300	s
$\text{C}-\text{X}$ Fluoride	1400-1000	s
Chloride	800-600	s
Bromide, iodide	> 600	s

**Table IR.2** Base Values for Absorptions of Bonds

$\text{OH}$	$3600\text{ cm}^{-1}$	$\text{C}\equiv\text{C}$	$2150\text{ cm}^{-1}$
$\text{NH}$	$3500\text{ cm}^{-1}$	$\text{C}=\text{O}$	$1715\text{ cm}^{-1}$
$\text{CN}$	$3000\text{ cm}^{-1}$	$\text{C}=\text{C}$	$1650\text{ cm}^{-1}$
$\text{C}\equiv\text{N}$	$2250\text{ cm}^{-1}$	$\text{C}-\text{O}$	$1100\text{ cm}^{-1}$