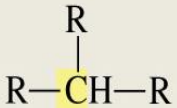
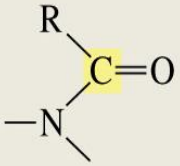
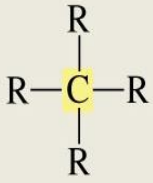
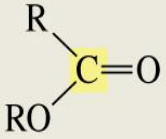
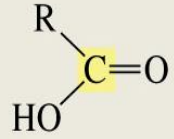
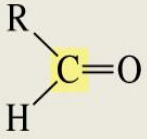
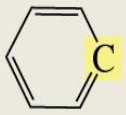
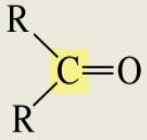
Table 14.4 Approximate Values of Chemical Shifts for ^{13}C NMR

Type of carbon	Approximate chemical shift (ppm)	Type of carbon	Approximate chemical shift (ppm)
$(CH_3)_4Si$	0	C—I	0–40
R—CH_3	8–35	C—Br	25–65
R—CH_2—R	15–50	C—Cl C—N C—O	35–80 40–60 50–80
	20–60		165–175
	30–40		165–175
≡C	65–85		175–185
=C	100–150		190–200
	110–170		205–220

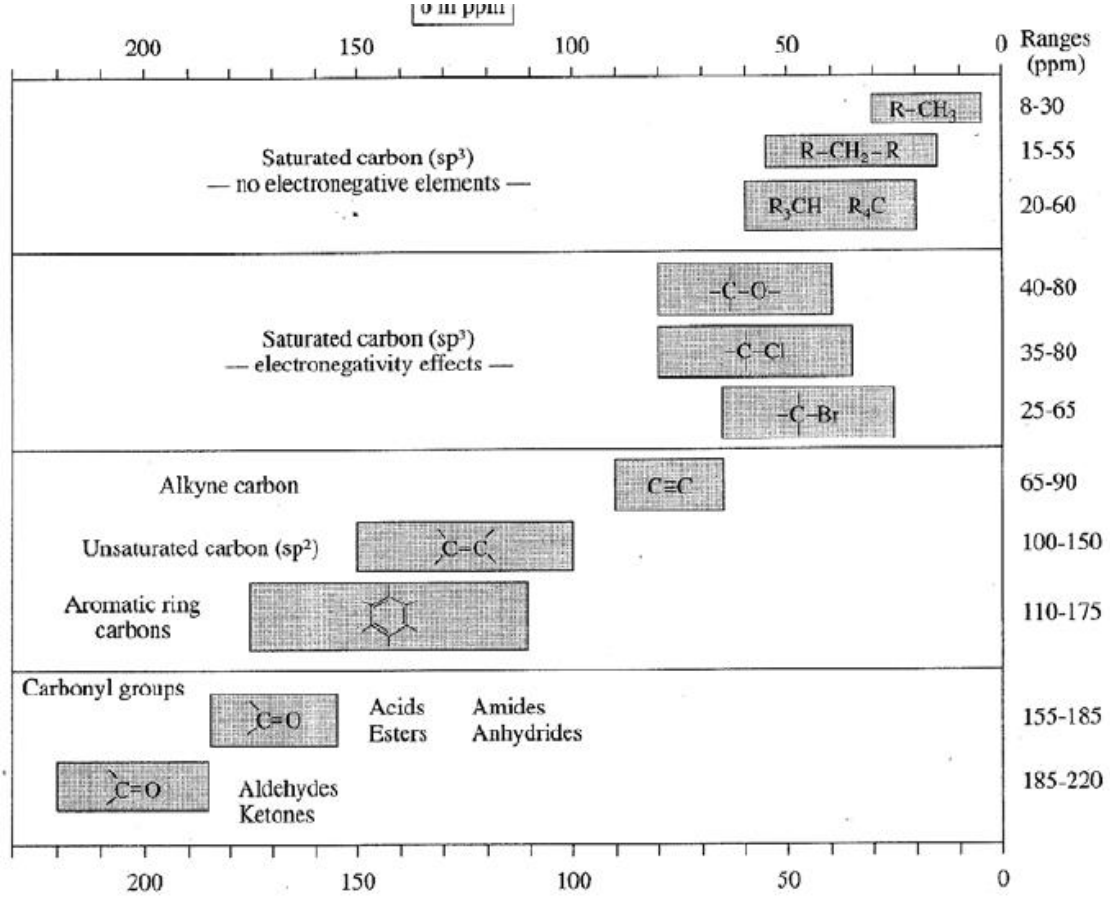
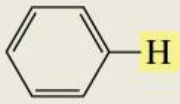
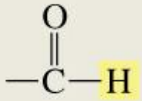
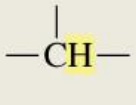
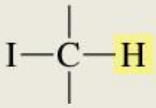
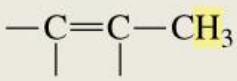
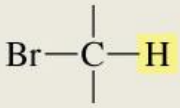
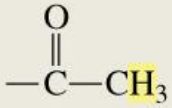
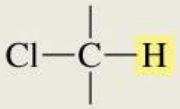
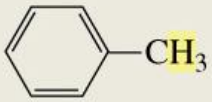
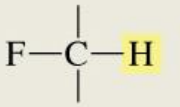
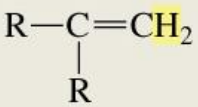
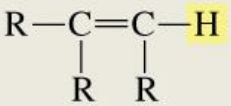
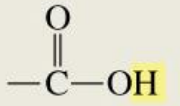
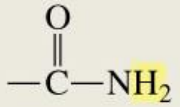


Table 14.3 Approximate Values of Coupling Constants

Approximate value of J_{ab} (Hz)		Approximate value of J_{ab} (Hz)	
H_a H_b —C—C—	7	H_a C=C H_b	15 (trans)
H_a H_b —C—C—C—	0	H_a H_b C=C	10 (cis)
H_a C=C H_b	2 (geminal coupling)	H_a C=C C H_b	1 (long-range coupling)

Table 14.1 Approximate Values of Chemical Shifts for ^{1}H NMR[a]

Type of proton	Approximate chemical shift (ppm)	Type of proton	Approximate chemical shift (ppm)
$(CH_3)_4Si$	0		6.5–8
$-CH_3$	0.9		
$-CH_2-$	1.3		9.0–10
	1.4		2.5–4
	1.7		
			2.5–4
	2.1		
			3–4
	2.3		
			4–4.5
$-C\equiv C-H$	2.4		
$R-O-CH_3$	3.3	RNH_2	Variable, 1.5–4
	4.7	ROH	Variable, 2–5
		ArOH	Variable, 4–7
	5.3		Variable, 10–12
			Variable, 5–8

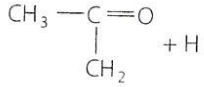
[a]The values are approximate because they are affected by neighboring substituents.

Tabela 2.3 Tabela de correlação simplificada

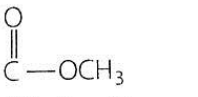
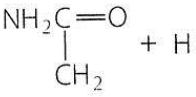
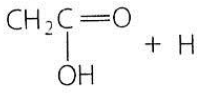
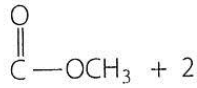
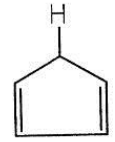
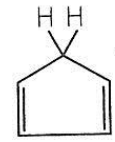
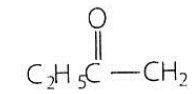
Tipo de Vibração		Frequência (cm^{-1})	Intensidade	Página de referência
C — H	Alcanos			
	(estiramento)	3000–2850	s	31
	$—CH_3$			
	(dobramento)	1450 e 1375	m	
	$—CH_2—$			
	(dobramento)	1465	m	
	Alcenos			
	(estiramento)	3100–3000	m	33
	(dobramento fora do plano)	1000–3000	s	
	Aromáticos			
	(estiramento)	3150–3050	s	43
	(dobramento fora do plano)	900–690	s	
	Alcino			
	(estiramento)	ca. 3300	s	35
	Aldeído	2900–2800	w	56
		2800–2700	w	
C — C	Alcano	Inútil para interpretação		
C = C	Alceno	1680–1600	m–w	33
	Aromático	1600 e 1475	m–w	43
C ≡ C	Alcino	2250–2100	m–w	35
C = O	Aldeído	1740–1720	s	56
	Cetona	1725–1705	s	58
	Ácido carboxílico	1725–1700	s	62
	Éster	1750–1730	s	64
	Amida	1680–1630	s	70
	Anidrido	1810 e 1760	s	73
	Cloreto ácido	1800	s	72
C — O	Alcoóis, éteres, ésteres, ácidos carboxílicos, anidridos	1300–1000	s	47, 50, 62, 64 e 73
O — H	Alcoóis, fenóis			
	Livres	3650–3600	m	47
	Ligação de H	3400–3200	m	47
	Ácidos carboxílicos	3400–2400	m	62
N — H	Aminas e amidas primárias e secundárias			
	(estiramento)	3500–3100	m	74
	(dobramento)	1640–1550	m–s	74
C — N	Aminas	1350–1000	m–s	74
C = N	Iminas e oximas	1690–1640	w–s	77
C ≡ N	Nitrilas	2260–2240	m	77
X = C = Y	Alenos, cetenas, isocianatos, isotiocianatos	2270–1940	m–s	77
N = O	Nitro ($R—NO_2$)	1550 e 1350	s	79
S — H	Mercaptanos	2550	w	81
S = O	Sulfóxidos	1050	s	81
	Sulfonas, cloretos de sulfonila, sulfatos, sulfonamidas	1375–1300 e 1350–1140	s	82
C — X	Fluoreto	1400–1000	s	85
	Cloreto	785–540	s	85
	Brometo, iodeto	< 667	s	85

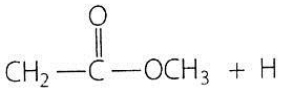
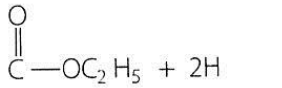
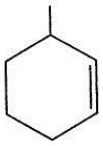
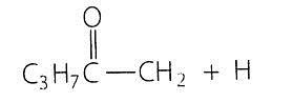
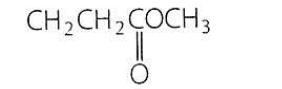
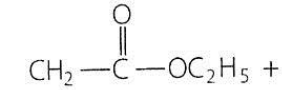
Íons Fragmentos Comuns com Massa abaixo de 105[a]

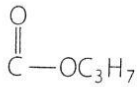
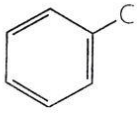
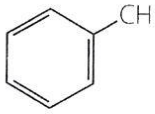
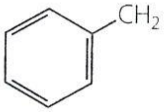
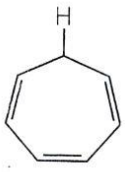
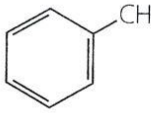
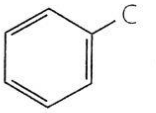
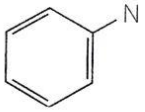
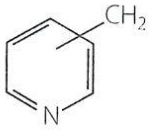
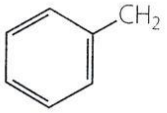
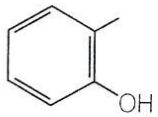
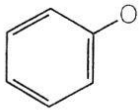
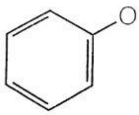
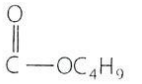
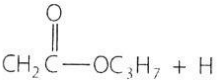
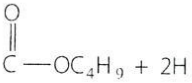
m/z	Íons
14	CH_2
15	CH_3
16	O
17	OH
18	H_2O
	NH_4
19	F
	H_3O
26	$C\equiv N$
27	C_2H_3
28	C_2H_4
	CO
	N_2 (ar)
	$CH{=}NH$
29	C_2H_5
	CHO
30	CH_2NH_2
	NO
31	CH_2OH
	OCH_3
32	O_2 (ar)
33	SH
	CH_2F
34	H_2S
35	Cl
36	HCl
39	C_3H_3
40	$C\equiv N$
41	C_3H_5
	$CH_2C{=}H + H$
	C_2H_2NH
42	C_3H_6
43	C_3H_7
	$CH_3C{=}O$
	C_2H_5N

m/z	Íons
44	$CH_2CH{=}O + H$
	CH_3CHNH_2
	CO_2
	$NH_2C{=}O$
	$(CH_3)_2N$
45	CH_3CHOH
	CH_2CH_2OH
	CH_2OCH_3
	
	$CH_3CH{-}O + H$
46	NO_2
47	CH_2SH
	CH_3S
48	$CH_3S + H$
49	CH_2Cl
51	CHF_2
	C_4H_3
53	C_4H_5
54	$CH_2CH_2C\equiv N$
55	C_4H_7
	$CH_2{=}CHC{=}O$
56	C_4H_8
57	C_4H_9
	$C_2H_5C{=}O$
58	
	$C_2H_5CHNH_2$
	$(CH_3)_2NHCH_2$
	$C_2H_5NHCH_2$
	C_2H_2S

[a] *Adaptado, com permissão, de SILVERSTEIN, R. M.; WEBSTER, F. X.* Spectrometric identification of organic compounds. *6. ed. Nova York: John Wiley & Sons, 1998.*

m/z	Íons
59	$(CH_3)_2COH$
	$CH_2OC_2H_5$
	
	
	CH_3OCHCH_3
	CH_3CHCH_2OH
60	
	CH_2ONO
61	
	CH_2CH_2SH
	CH_2SCH_3
65	 (ou C_5H_5)
66	 (ou C_5H_6)
67	C_5H_7
68	$CH_2CH_2CH_2C{\equiv}N$
69	C_5H_9
	CF_3
	$CH_3CH{=}CHC{=}O$
	$CH_2{=}C(CH_3)C{=}O$
70	C_5H_{10}
71	C_5H_{11}
	$C_3H_7C{=}O$
72	
	$C_3H_7CHNH_2$
	$(CH_3)N{=}C{=}O$
	$C_2H_5NHCHCH_3$ e isômeros
73	Homólogos de 59

m/z	Íons
74	
75	
	$CH_2SC_2H_5$
	$(CH_3)_2CSH$
	$(CH_3O)_2CH$
77	C_6H_5
78	$C_6H_5 + H$
79	$C_6H_5 + 2H$
	Br
80	$CH_3SS + H$
81	C_6H_9 
82	$CH_2CH_2CH_2CH_2C{\equiv}N$
	CCl_2
	C_6H_{10}
83	C_6H_{11}
	$CHCl_2$
85	C_6H_{13}
	$C_4H_9C{=}O$
	$CClF_2$
86	
	$C_4H_9CHNH_2$ e isômeros
87	
	Homólogos de 73
	
88	

m/z	Íons
89	 + 2H 
90	CH_3CHONO_2 
91	 ou   + H  + 2H $(CH_2)_4Cl$ 
92	  + H
93	CH_2Br  C_7H_9 
94	 + H
96	$CH_2CH_2CH_2CH_2CH_2C{\equiv}N$
97	C_7H_{13}
99	C_7H_{15} $C_6H_{11}O$
100	 + H $C_5H_{11}CHNH_2$
101	
102	 + H
103	 + 2H $C_5H_{11}S$ $CH(OCH_2CH_3)_2$
104	$C_2H_5CHONO_2$
105