Tabela com massas exatas dos isótopos

Table I. Exact Masses of Isotopes

Element	Atomic Weight	Nuclide	Mass
Hydrogen	1.00797	^{1}H	1.00783
		D (^{2}H)	2.01410
Carbon	12.01115	^{12}C	12.00000 (std)
		^{13}C	13.00336
Nitrogen	14.0067	^{14}N	14.0031
		^{15}N	15.0001
Oxygen	15.9994	^{16}O	15.9949
		^{17}O	16.9991
		^{18}O	17.9992
Fluorine	18.9984	^{19}F	18.9984
Silicon	28.086	^{28}Si	27.9769
		^{29}Si	28.9765
		^{30}Si	29.9738
Phosphorus	30.974	^{31}P	30.9738
Sulfur	32.064	^{32}S	31.9721
		^{33}S	32.9715
		^{34}S	33.9679
Chlorine	35.453	^{35}Cl	34.9689
		^{37}Cl	36.9659
Bromine	79.909	^{79}Br	78.9183
		^{81}Br	80.9163
Iodine	126.904	^{127}I	126.9045

Abundância natural de alguns isótopos importantes para a Química Orgânica

Table II. Relative Isotope Abundances of Common Elements

Elements	Abundance					
Carbon	^{12}C	100	^{13}C	1.08		
Hydrogen	^{1}H	100	^{2}H	0.016		
Nitrogen	^{14}N	100	^{15}N	0.38		
Oxygen	^{16}O	100	^{17}O	0.04	^{18}O	0.20
Fluorine	^{19}F	100				
Silicon	^{28}Si	100	^{29}Si	5.10	^{30}Si	3.35
Phosphorus	^{31}P	100				
Sulfur	^{32}S	100	^{33}S	0.78	^{34}S	4.40
Chlorine	^{35}Cl	100	^{37}Cl	32.5		
Bromine	^{79}Br	100	^{81}Br	98.0		
Iodine	^{127}I	100				

Intensidade dos picos (relativo ao M^+) para combinações de Cl e Br

Table III. Intensities of Isotope Peaks (Relative to the Molecular Ion) for Combinations of Bromine and Chlorine

Halogen Present	% $M+2$	% $M+4$	% $M+6$	% $M+8$	% $M+10$	% $M+12$
Br	97.9					
Br_2	195.0	95.5				
Br_3	293.0	286.0	93.4			
Cl	32.6					
Cl_2	65.3	10.6				
Cl_3	97.8	31.9	3.47			
Cl_4	131.0	63.9	14.0	1.15		
Cl_5	163.0	106.0	34.7	5.66	0.37	
Cl_6	196.0	161.0	69.4	17.0	2.23	0.11
BrCl	130.0	31.9				
Br_2Cl	228.0	159.0	31.2			
Cl_2Br	163.0	74.4	10.4			

Padrões de diferentes combinações isotópicas de cloros e bromos

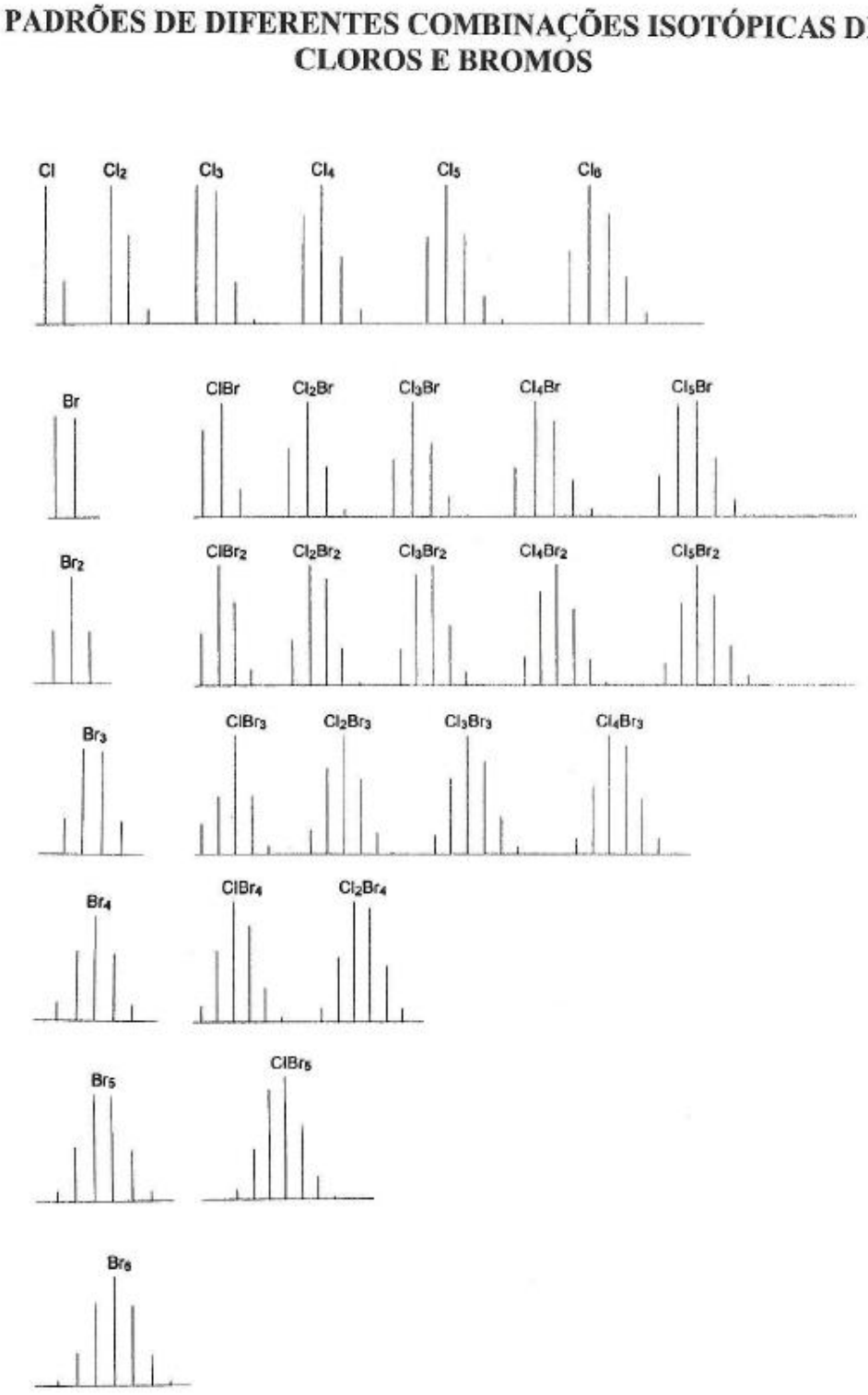


FIGURE 6.22 Patterns of different isotopic combinations of Cl and Br. All signals are separated by 2 amu.

Apendice B (Fragmentos iônicos mais comumente encontrados)

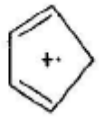
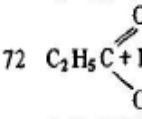
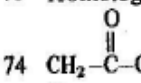
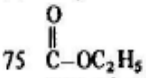
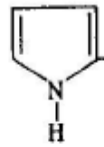
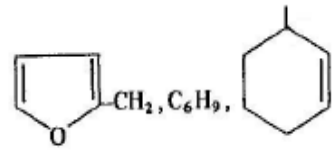
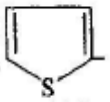
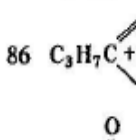
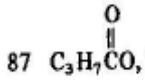
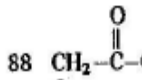
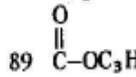
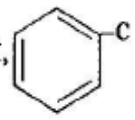
FRAGMENTOS IÔNICOS COMUNS

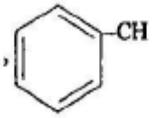
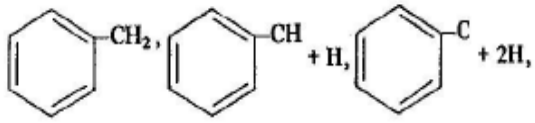
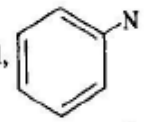
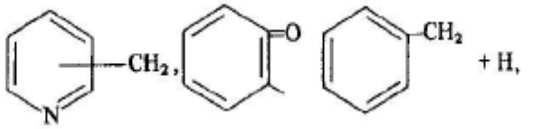
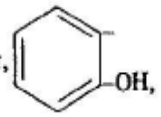
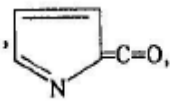
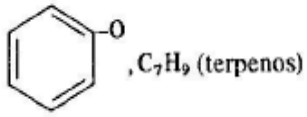
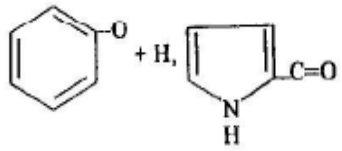
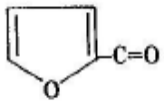
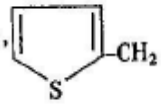
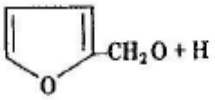
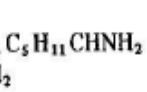
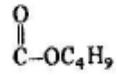
Nem todos os termos das séries homólogas e isoméricas são dados aqui. A lista é mais sugestiva do que exaustiva. Os suplementos recomendados são o Apêndice II de Hamming e Foster,[10f] a Tabela A-7 de *McLafferty's Interpretative Book*[10c] e dados de íons de alta resolução de McLafferty.

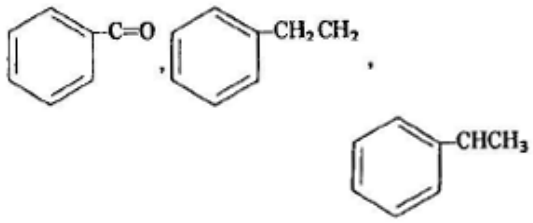
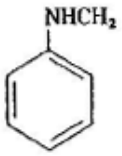
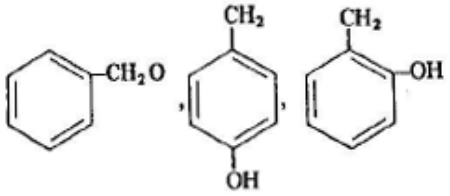
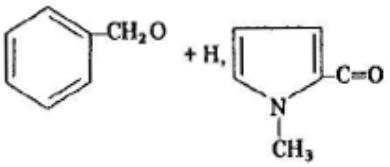
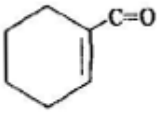
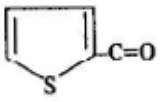
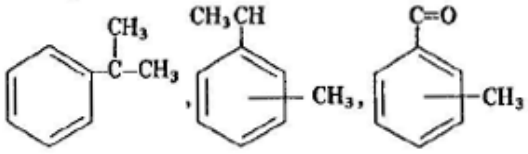
m/e	Íons*
14	CH_2
15	CH_3
16	O
17	OH
18	H_2O, NH_4
19	F, H_3O
26	$C{\equiv}N$
27	C_2H_3
28	C_2H_4, CO, N_2 (ar), CH=NH
29	C_2H_5, CHO
30	CH_2NH_2, NO
31	CH_2OH, OCH_3
32	O_2 (Ar)
33	SH, CH_2F
34	H_2S
35	Cl
36	HCl
39	C_3H_3
40	$CH_2C{=}N$, Ar(Ar)
41	C_3H_5, $CH_2C{=}N + H$, C_2H_2NH
42	C_3H_6
43	C_3H_7, $CH_3C{=}O$, C_2H_5N
44	$CH_2C{=}O + H$, CH_3CHNH_2, CO_2, $NH_2C{=}O$, $(CH_3)_2N$
45	$CHOH$, CH_2CH_2OH, CH_2OCH_3, $C(=O)OH$, $CH_3CH{-}O + H$

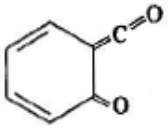
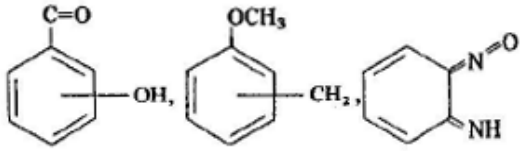
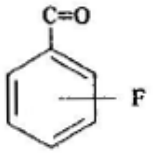
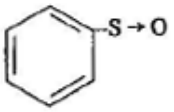
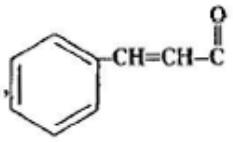
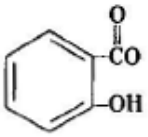
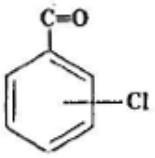
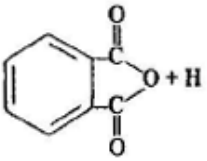
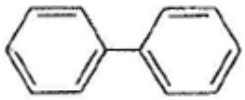
m/e	Íons
46	NO_2
47	CH_2SH, CH_3S
48	$CH_3S + H$
49	CH_2Cl
51	CHF_2
53	C_4H_5
54	$CH_2CH_2C{\equiv}N$
55	C_4H_7, $CH_2{=}CHC{=}O$
56	C_4H_8
57	C_4H_9, $C_2H_5C{=}O$
58	$CH_3{-}C(=O){+}H$, $C_2H_5CHNH_2$, $(CH_3)_2NCH_2$, $C_2H_5NHCH_2$, C_2H_2S
59	$(CH_3)_2COH$, $CH_2OC_2H_5$, $C(=O){-}OCH_3$, $NH_2C(=O){+}H$, CH_3OCHCH_3, CH_3CHCH_2OH
60	$CH_2C(=O){+}H$, CH_2ONO
61	$C(=O){-}OCH_3 + 2H$, CH_2CH_2SH, CH_2SCH_3
65	 $\equiv C_5H_5$

*Os íons indicados como um fragmento + nH (n = 1, 2, 3,...) são íons que se originam de um rearranjo envolvendo transferência de hidrogênio.

m/e	Íons
66	 ≡ 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	 + H, $C_3H_7CHNH_2$, $(CH_3)_2N{=}C{=}O$, $C_2H_5NHCHCH_3$, e isômeros
73	Homólogos de 59
74	 + H
75	 + 2H, $CH_2SC_2H_5$, $(CH_3)_2CSH$, $(CH_3O)_2CH$
77	C_6H_5
78	C_6H_5 + H
79	C_6H_5 + 2H, Br
80	 CH_2, CH_3SS + H
81	 CH_2, 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	 + H, $C_4H_9CHNH_2$, e isômeros.
87	 CO, homólogos de 73, $CH_2CH_2COCH_3$ 
88	 + H
89	 + 2H, 

m/e	Íons
90	CH_3CHONO_2, 
91	 + H, + 2H,
	$(CH_2)_4Cl$, 
92	 + H,
93	CH_2Br,  C_7H_9,   , C_7H_9 (terpenos)
94	 + H,
95	
96	$CH_2CH_2CH_2CH_2CH_2C{\equiv}N$
97	C_7H_{13}, 
98	 + H
99	C_7H_{15}, $C_6H_{11}O$
100	 + H, $C_5H_{11}CHNH_2$
101	

m/e	Ions
102	$CH_2C(=O)-OC_3H_7 + H$
103	$C(=O)-OC_4H_9 + 2H$, $C_5H_{11}S$, $CH(OCH_2CH_3)_2$
104	$C_2H_5CHONO_2$
105	
106	
107	
108	
109	
111	
119	CF_3CF_2, 

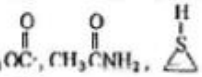
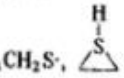
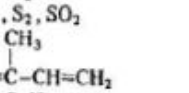
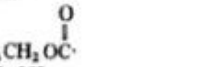
m/e	Ions
120	
121	
	C_9H_{13} (terpenos)
123	
125	
127	I
131	C_3F_5, 
135	$(CH_2)_4Br$
138	
139	
149	
154	

Apendice C (Fragmentos eliminados com facilidade)

FRAGMENTOS ELIMINADOS COM FACILIDADE

Esta lista é mais sugestiva do que completa. Ela deverá ser usada em conjunto com o Apêndice B. Os suplementos recomendados são a Tabela 5-19 de Hamming e Foster[10f] e a Tabela A-5 de McLafferty.[10c]

Íons moleculares menos	Fragmentos eliminados
1	H·
15	CH_3·
17	HO·
18	H_2O
19	F·
20	HF
26	CH≡CH, ·C≡N
27	CH_2=CH·, HC≡N
28	CH_2=CH_2, CO, (HCN + H)
29	CH_3CH_2·, ·CHO
30	NH_2CH_2·, CH_2O, NO
31	·OCH_3, ·CH_2OH, CH_3NH_2
32	CH_3OH, S
33	HS·, (·CH_3 e H_2O)
34	H_2S
35	Cl·
36	HCl, $2H_2O$
37	H_2Cl (ou HCl + H)
38	C_3H_2·, C_2N, F_2
39	C_3H_3, HC_2N
40	CH_3C≡CH
41	CH_2=$CHCH_2$
42	CH_2=$CHCH_3$, CH_2=C=O,  , NCO, $NCNH_2$
43	C_3H_7·, , CH_2=CH–O·, [CH_3· e CH_2=CH_2], HCNO
44	CH_2=CHOH, CO_2, N_2O, $CONH_2$, $NHCH_2CH_3$
45	CH_3CHOH, CH_3CH_2O·, CO_2H, $CH_3CH_2NH_2$
46	[H_2O e CH_2=CH_2], CH_3CH_2OH, ·NO_2
47	CH_3S·
48	CH_3SH, SO, O_3
49	·CH_2Cl
51	·CHF_2

Íons moleculares menos	Fragmentos eliminados
52	C_4H_4, C_2N_2
53	C_4H_5
54	CH_2=CH–CH=CH_2
55	CH_2=$CHCHCH_3$
56	CH_2=$CHCH_2CH_3$, CH_3CH=$CHCH_3$, 2CO
57	C_4H_9·
58	·NCS, (NO + CO), CH_3COCH_3
59	
60	C_3H_7OH
61	
62	[H_2S e CH_2=CH_2]
63	·CH_2CH_2Cl
64	C_5H_4, S_2, SO_2
68	
69	CF_3·, C_5H_9·
71	C_5H_{11}·
73	
74	C_6H_9OH
75	C_6H_3
76	C_6H_4, CS_2
77	C_6H_5, CS_2H
78	C_6H_6, CS_2H_2, C_5H_4N
79	Br·, C_5H_5N
80	HBr
85	·$CClF_2$
100	CF_2=CF_2
119	CF_2–CF_2·
122	C_6H_5COOH
127	I·
128	HI