

APPENDIX C COMMON FRAGMENTS LOST

This list is suggestive rather than comprehensive. It should be used in conjunction with Appendix B, Table 5-19 of Hamming and Foster (1972) and Table A-5 of McLafferty (1993) are

recommended as supplements. All of these fragments are lost as neutral species.

Molecular Ion Minus	Fragment Lost (Inference Structure)
1	H·
2	2H·
15	CH ₃ ·
16	O (ArNO ₂ , amine oxides, sulfoxides); ·NH ₂ (carboxamides, sulfonamides)
17	HO·
18	H ₂ O (alcohols, aldehydes, ketones)
19	F·
20	HF
26	CH≡CH, ·CH≡N
27	CH ₂ =CH·, HC≡N (aromatic nitrites, nitrogen heterocycles)
28	CH ₂ =CH ₂ , CO, (quinones) (HCN + H)
29	CH ₃ CH ₂ ·, (ethyl ketones, ArCH ₂ CH ₂ CH ₃), ·CHO
30	NH ₂ CH ₂ ·, CH ₂ O (ArOCH ₃), NO (ArNO ₂), C ₂ H ₆
31	·OCH ₃ (methyl esters), ·CH ₂ OH, CH ₃ NH ₂
32	CH ₃ OH, S
33	HS· (thiols), (·CH ₃ and H ₂ O)
34	H ₂ S (thiols)
35	Cl·
36	HCl, 2H ₂ O
37	H ₂ Cl (or HCl + H)
38	C ₃ H ₂ , C ₂ N, F ₂
39	C ₃ H ₃ , HC ₂ N
40	CH ₃ C≡CH
41	CH ₂ =CHCH ₂ ·
42	CH ₂ =CHCH ₃ , CH ₂ =C=O, H ₂ C ^H —CH ₂ , NCO, NCNH ₂
43	C ₃ H ₇ · (propyl ketones, ArCH ₂ —C ₃ H ₇), CH ₃ C· (methyl ketones, CH ₃ C ^O G, where G = various functional groups), CH ₂ =CH—O·, (CH ₃ · and CH ₂ =CH ₂), HCNO
44	CH ₂ =CHOH, CO ₂ (esters, anhydrides), N ₂ O, CONH ₂ , NHCH ₂ CH ₃
45	CH ₃ CHOH, CH ₃ CH ₂ O· (ethyl esters), CO ₂ H, CH ₃ CH ₂ NH ₂
46	(H ₂ O and CH ₂ =CH ₂), CH ₃ CH ₂ OH, ·NO ₂ (ArNO ₂)
47	CH ₃ S·
48	CH ₃ SH, SO (sulfoxides), O ₃
49	·CH ₂ Cl
51	·CHF ₂
52	C ₄ H ₄ , C ₂ N ₂
53	C ₄ H ₅
54	CH ₂ =CH—CH=CH ₂
55	CH ₂ =CHCHCH ₃

APPENDIX C (Continued)

Molecular Ion Minus	Fragment Lost (Inference Structure)
56	$\text{CH}_2=\text{CHCH}_2\text{CH}_3$, $\text{CH}_3\text{CH}=\text{CHCH}_3$, 2CO
57	$\text{C}_4\text{H}_9\cdot$ (butyl ketones), $\text{C}_2\text{H}_5\text{CO}$ (ethyl ketones, $\text{EtC}=\text{OG}$, G = various structural units)
58	$\cdot\text{NCS}$, ($\text{NO} + \text{CO}$), CH_3COCH_3 , C_4H_{10}
59	$\begin{array}{c} \text{O} \quad \text{O} \quad \text{H} \\ \parallel \quad \parallel \quad \\ \text{CH}_3\text{OC}\cdot, \text{CH}_3\text{CNH}_2, \triangle \\ \text{S}\cdot \end{array}$
60	$\text{C}_3\text{H}_7\text{OH}$, $\text{CH}_2=\text{C}(\text{OH})_2$ (acetate esters)*
61	$\begin{array}{c} \text{H} \\ \\ \text{CH}_3\text{CH}_2\text{S}\cdot, \triangle \\ \text{S}\cdot \end{array}$
62	(H_2S and $\text{CH}_2=\text{CH}_2$)
63	$\cdot\text{CH}_2\text{CH}_2\text{Cl}$
64	C_3H_8 , S_2 , SO_2
68	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_2=\text{C}-\text{CH}=\text{CH}_2 \end{array}$
69	$\text{CF}_3\cdot$, $\text{C}_3\text{H}_9\cdot$
71	$\text{C}_5\text{H}_{11}\cdot$
73	$\begin{array}{c} \text{O} \\ \parallel \\ \text{CH}_3\text{CH}_2\text{OC}\cdot \end{array}$
74	$\text{C}_3\text{H}_7\text{OH}$
75	C_6H_5
76	C_6H_4 , CS_2
77	C_6H_5 , CS_2H
78	C_6H_6 , CS_2H_2 , $\text{C}_5\text{H}_4\text{N}$
79	$\text{Br}\cdot$, $\text{C}_5\text{H}_5\text{N}$
80	HBr
85	$\cdot\text{CClF}_2$
100	$\text{CF}_2=\text{CF}_2$
119	$\text{CF}_3-\text{CF}_2\cdot$
122	$\text{C}_6\text{H}_5\text{COOH}$
127	$\text{I}\cdot$
128	HI

* McLafferty rearrangement.