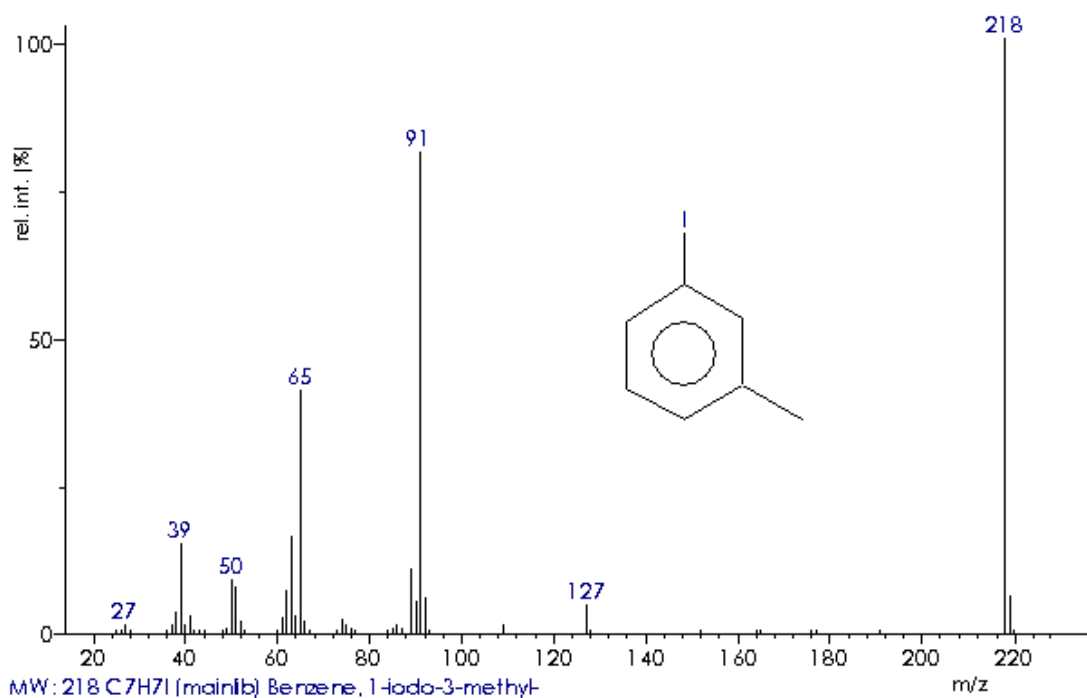


Answer 6.14

Identify the unknown from its 70 eV EI mass spectrum.



The molecular ion, $M^{+} = 218$ (base peak), is very stable, and its even mass indicates 0, 2, 4, ... nitrogen atoms.

The isotopic pattern shows no Cl, Br, Si or S.

From the ^{13}C -peak (7 %, use a ruler) we estimate only 6–7 carbons.

m/z 127	$[M-91]$, $[M-C_7H_7]^+$?
m/z 91	$[M-127]$, $[M-I]^+ \equiv [C_7H_7]^+$?
m/z 65	$[M-127-26]$, $[C_5H_5]^+$?
m/z 51	$[C_4H_3]^+$, aromatic fragment
m/z 50	$[C_4H_2]^+$, aromatic fragment „–1 u“
m/z 39	$[C_3H_3]^+$, aromatic fragment

The molecule must have a simple structure. Loss of 127 u corresponds to I $^{\bullet}$ which is also consistent with a ^{13}C -peak of only 7 % despite of $M^{+} = 218$.

The series m/z 39, 50, 51, 65, (76), 91 clearly points to $[C_7H_7]^+$ and its fragment ions.

The molecular formula is C₇H₇I; $r+d = 7 - 4 + 1 = 4$

The structure should not be benzylic, because m/z 50 indicates a doubly substituted ring. It cannot be decided whether the substituents stand *o*, *m*, or *p* to each other.

Fragmentation scheme:

