

MASS SPECTROMETRY (MS)

Exercise 1:

Determine the degree of unsaturation (IHD) for the hydrocarbons with the following molecular formulas:

(a) $C_{10}H_{16}$ HDI = 3

(b) C_7H_7NO HDI = 5

(c) C_8H_9ClO HDI = 4

Exercise 2:

An unknown substance shows a molecular ion peak at $m/z = 170$ with a relative intensity of 100. The $M + 1$ peak has an intensity of 13.2, and the $M + 2$ peak has an intensity of 1.00. What is the molecular formula of the unknown?

M^+ at $m/z = 170$ implies an even # of nitrogen
 M^+ peak it is the base peak, no recalculation necessary
 $M + 1$ peak 13.2 / 1.1 = 12; 12 carbons
 $M + 2$ peak 1.00% of M^+ ; no S, Cl, Br

$170 - (12)(12) = 26$ $C_{12}H_{26}$ is possible
cannot have two N MM exceeded
 $M + 2$ peak its presence might indicate oxygen
 $170 - (12)(12) - 16 = 10$ $C_{12}H_{10}O$

answer: $C_{12}H_{10}O$ (or $C_{12}H_{26}$)

Exercise 3:

An unknown hydrocarbon has a molecular ion peak at $m/z = 84$, with a relative intensity of 31.3. The $M + 1$ peak has a relative intensity of 2.06, and the $M + 2$ peak has a relative intensity of 0.08. What is the molecular formula for this substance?

M^+ at $m/z = 84$ implies an even # of nitrogen
 M^+ peak it is not the base peak, recalculation necessary
 M^+ 31.3 100%
 $M + 1$ 2.06 6.58% 6.58 / 1.1 = 5.98; 6 carbons
 $M + 2$ 0.08 0.25% no S, Cl, Br
 $84 - (6)(12) = 12$

answer: C_6H_{12}

Exercise 4:

An unknown substance has a molecular ion peak at $m/z = 107$, with a relative intensity of 100. The relative intensity of the $M + 1$ peak is 8.00, and the relative intensity of the $M + 2$ peak is 0.30. What is the molecular formula for this unknown?

M^+ at $m/z = 107$ implies an odd # of nitrogen
 M^+ peak it is the base peak, no recalculation necessary
 $M + 1$ peak $8.00 / 1.1 = 7.3$; 7 carbons
 $M + 2$ peak 0.30%; no S, Cl, Br
 $107 - (1)(14) - (7)(12) = 9$

answer: C_7H_9N

Exercise 5:

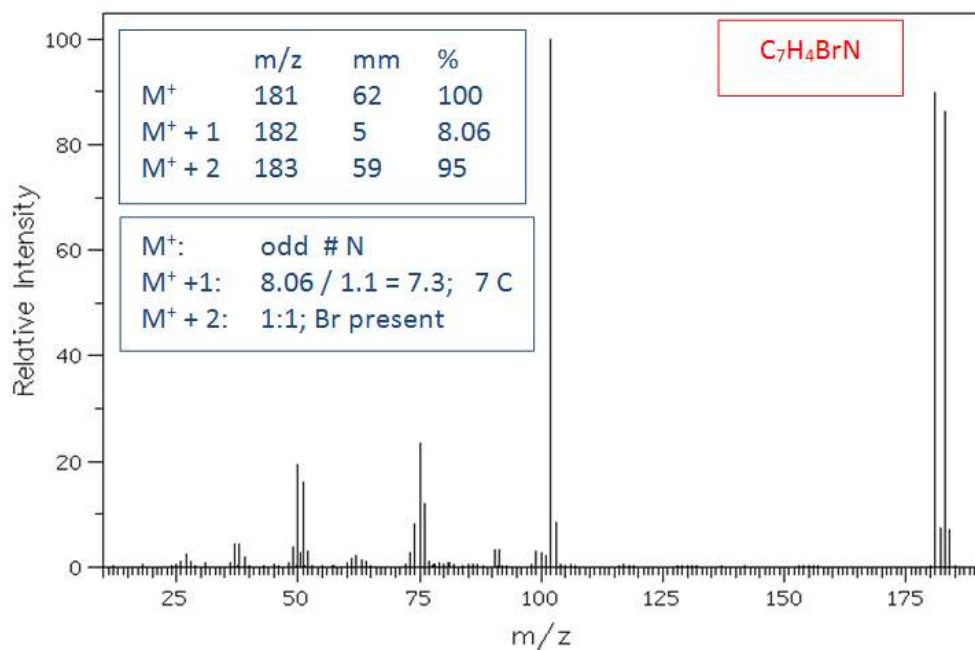
The mass spectral data of an unknown liquid are given below. What is the molecular formula of this unknown?

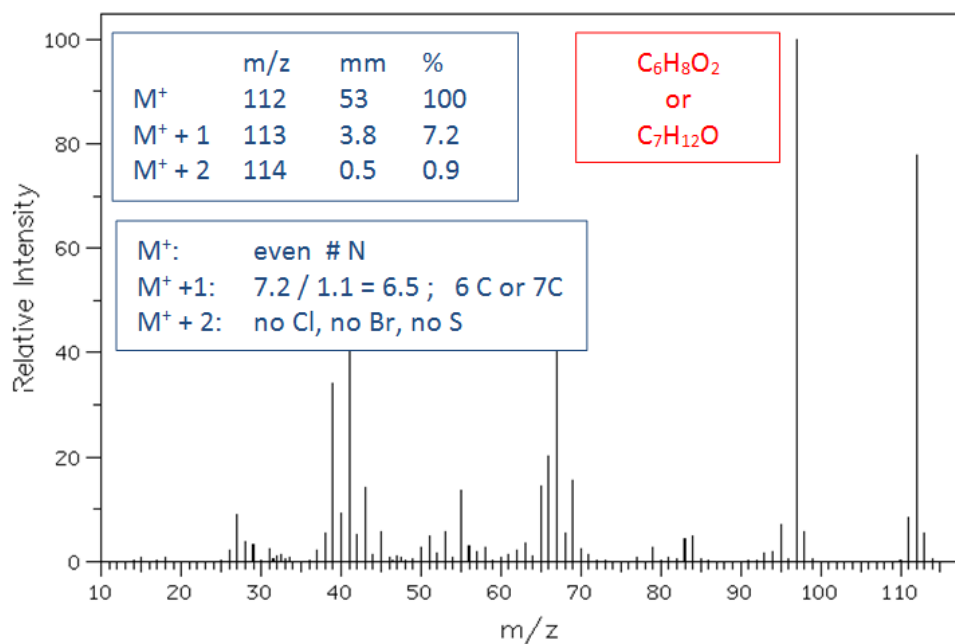
<u>m/z</u>	<u>intensity</u>					
78	23.6	(M^+)	M^+ at $m/z = 78$	implies an even # of nitrogen		
79	0.79		M^+ peak	it is not the base peak, recalculation necessary		
80	7.55		M^+ 23.6	100%		
81	0.25		$M + 1$ 0.79	3.35%	$3.35 / 1.1 = 3.05$; 3 carbons	
			$M + 2$ 7.55	32%	Cl is present	
						$78 - (3)(12) - 35 = 7$

answer: C_3H_7Cl

Exercise 6:

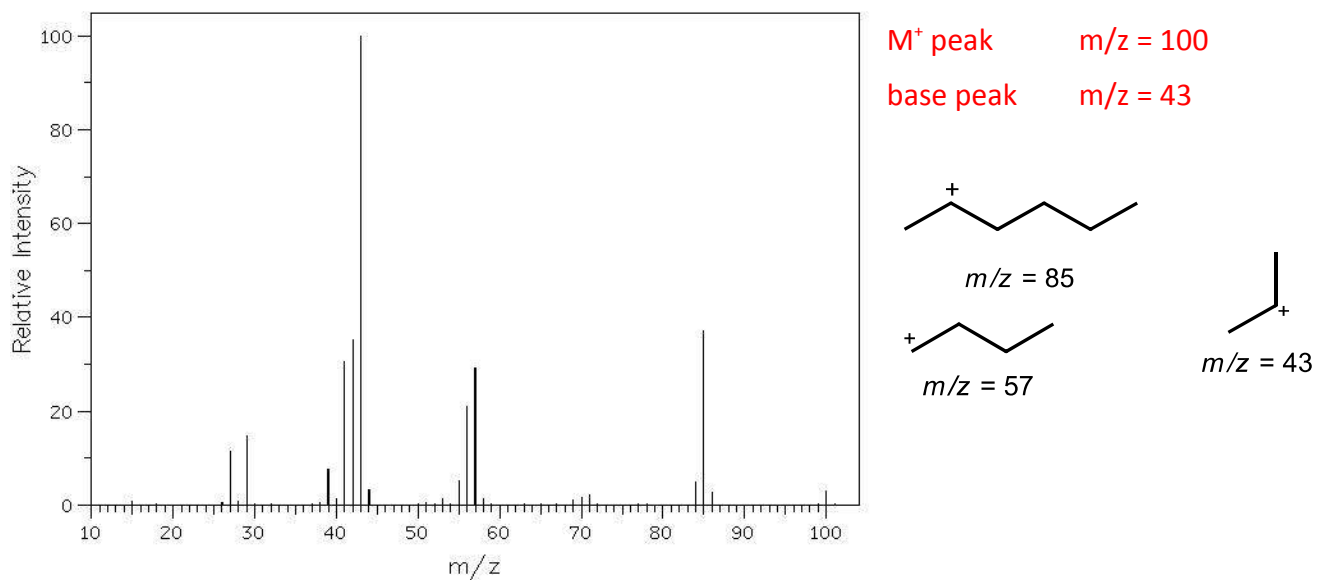
Propose a molecular formula for each mass spectrum:





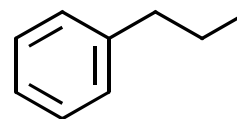
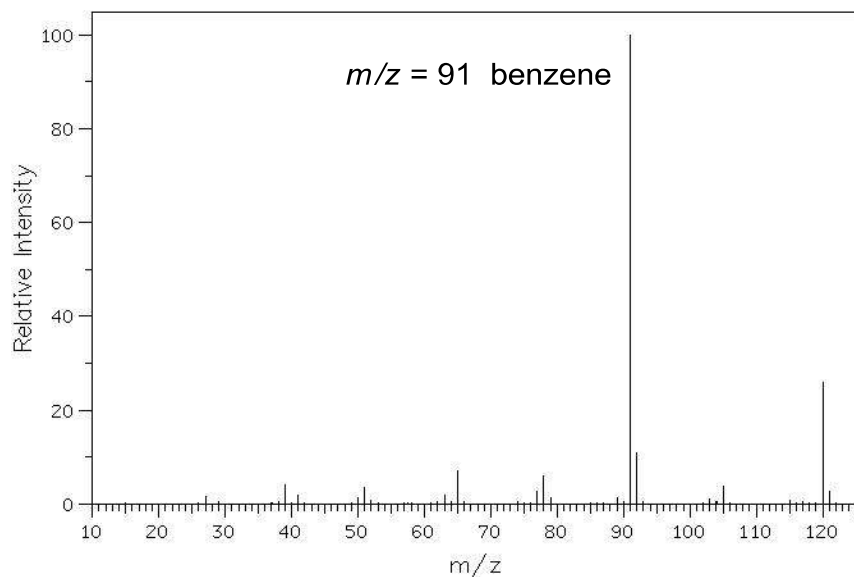
Exercise 7:

Look at the mass spectrum of 2-methylhexane. What is the m/z value of the M^+ peak and of the base peak? Give possible structures of the fragments giving rise to the large peaks at $m/z = 85$, 57, and 43.



Exercise 8:

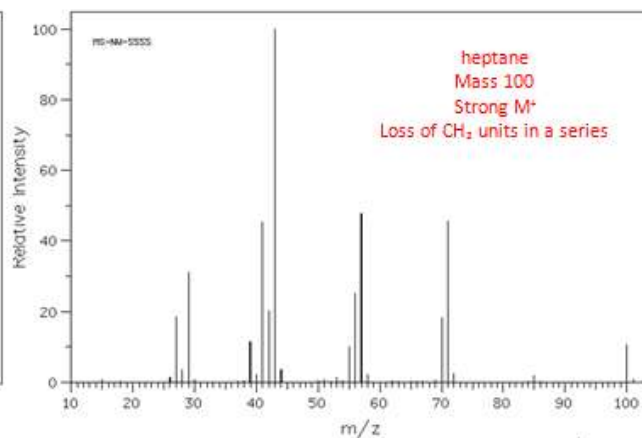
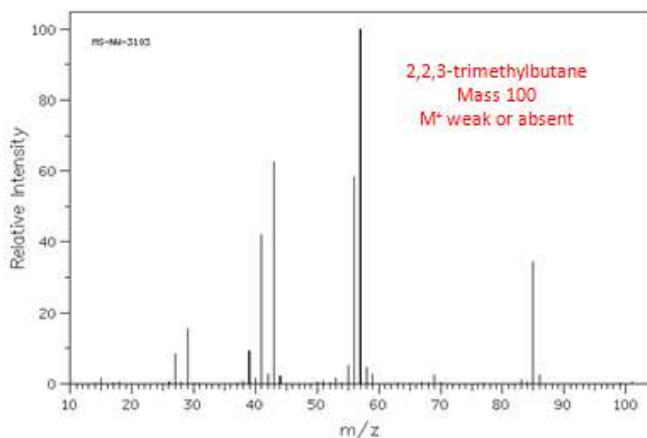
Give the structure of the molecule that gives the following mass spectrum.



mass = 120

Exercise 9:

The mass spectra of heptane and 2,2,3-trimethylbutane are given below. Which spectrum represents which compound? Explain.



Exercise 10:

Propose a structure for the compound having the following mass spectrum:

