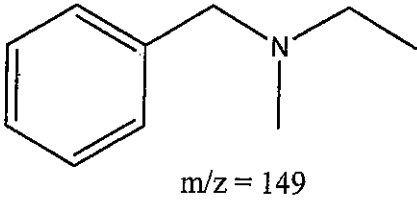
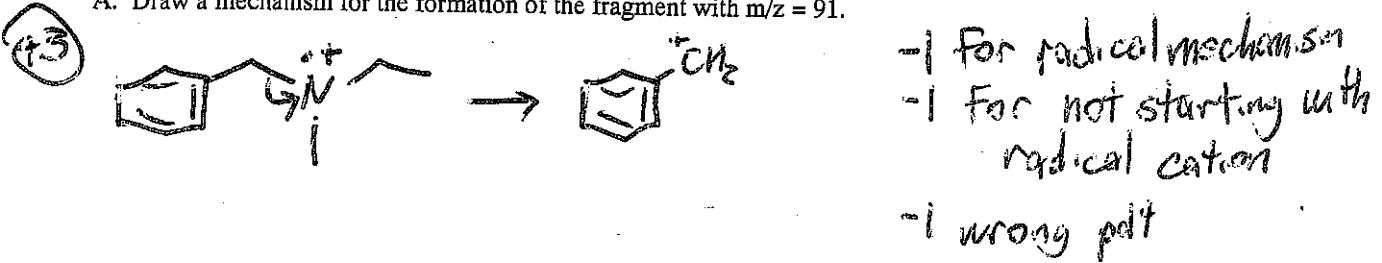


1. (10pts) The mass spectrum of N-benzyl-N-ethyl-N-methylamine contains a number of significant fragments.

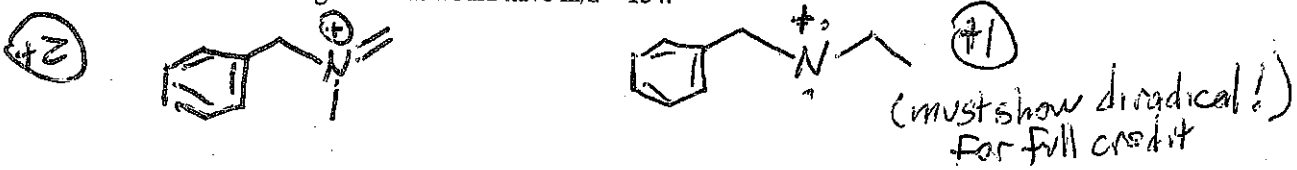


A. Draw a mechanism for the formation of the fragment with m/z = 91.



(+2) B. A fragment with m/z = 134 would involve loss of methyl.

C. Draw structures of a fragment that would have m/z = 134.



D. Draw a mechanism for the formation of the fragment with m/z = 72.



2. (2pts) The  $M^+$  peak of 1-chloro-2-bromopropane is m/z = 156 and has a relative abundance of 10. What would you expect the relative abundances be for the peaks at m/z 157 and 158? Show all work.

m/z	Rel. Abundance
156 ( $M^+$ )	1
157	0.03
158	1.31 (bonus)

(+2)

$$\frac{1.1}{98.9} (3 \text{ carbon}) = 0.033 \quad (1 \text{ relative abundance}) = 0.033$$

Bonus (+1)

$$^{37}\text{Cl} + ^{79}\text{Br} = .2423(.5069) = 0.123$$

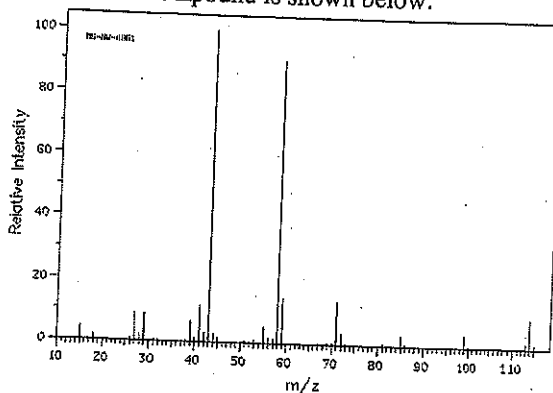
$$^{35}\text{Cl} + ^{81}\text{Br} = .7577(.4931) = .374$$

$$\text{total} = .123 + .374 = .50$$

$$\frac{x}{1} = \frac{.50}{.384}$$

$$M^+ = .7577(.5069) = .384$$

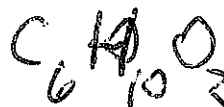
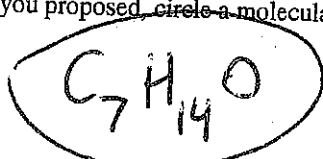
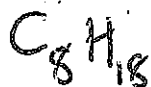
3. (8pts) The mass spectrum for an unknown compound is shown below:



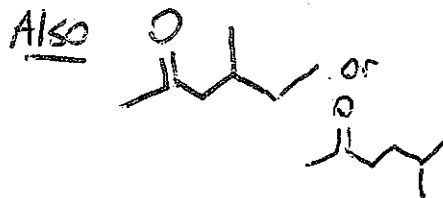
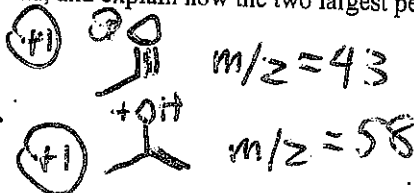
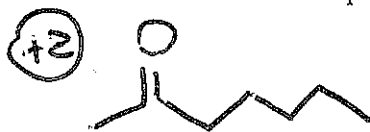
m/z	rel. abund.	m/z	rel. abund.	m/z	rel. abund.
15.0	4.2	42.0	3.0	59.0	14.8
18.0	1.5	43.0	100.0	71.0	14.0
27.0	8.9	44.0	2.4	72.0	3.9
28.0	2.0	45.0	1.4	85.0	3.3
29.0	8.7	53.0	1.0	99.0	4.1
39.0	6.7	55.0	5.1	113.0	1.7
40.0	1.0	56.0	1.5	114.0 (M <sup>+</sup> )	9.5
41.0	11.6	57.0	1.6	115.0	1.0
		58.0	90.6		

A. Use the Rule of 13 to propose THREE possible molecular formulae for this compound. This unknown has one degree of unsaturation. Of the three you proposed, circle a molecular formula consistent with this fact.

1 circle  
1 for each  
Formula



B. Propose a structure for the compound, and explain how the two largest peaks are consistent with this structure.



Other  $C_7H_{14}O$  compounds =  $+2$ , but no credit for fragments

The Natural Abundance of Isotopes Commonly Found in Organic Compounds

Element	Natural Abundance			
Carbon	$^{12}C$ : 98.89%	$^{13}C$ : 1.11%		
Hydrogen	$^1H$ : 99.99%	$^2H$ : 0.01%		
Nitrogen	$^{14}N$ : 99.64%	$^{15}N$ : 0.36%		
Oxygen	$^{16}O$ : 99.76%	$^{17}O$ : 0.04%	$^{18}O$ : 0.20%	
Sulfur	$^{32}S$ : 95.0%	$^{33}S$ : 0.76%	$^{34}S$ : 4.22%	$^{36}S$ : 0.02%
Chlorine	$^{35}Cl$ : 75.77%		$^{37}Cl$ : 24.23%	
Bromine	$^{79}Br$ : 50.69%		$^{81}Br$ : 49.31%	