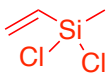


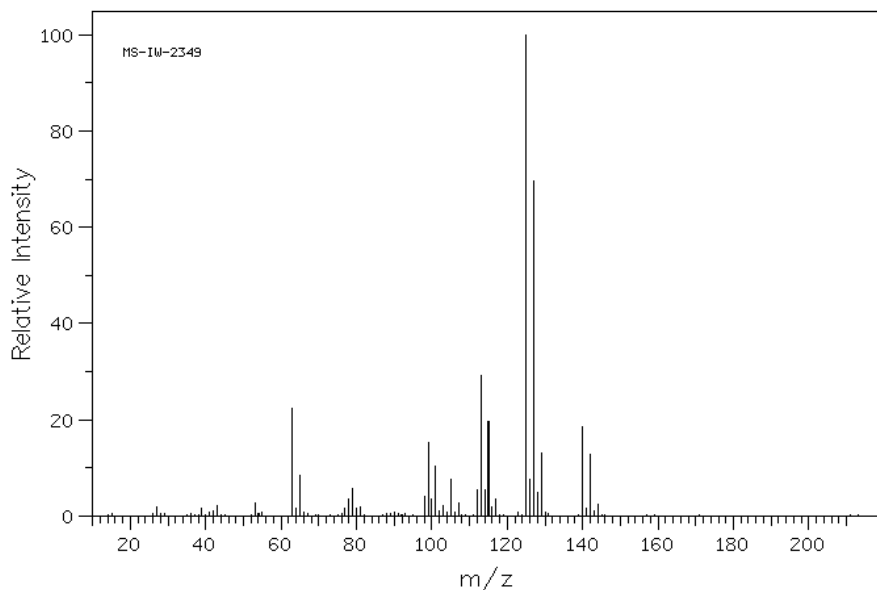
1. Answer the following questions about a molecule whose mass spectrometry data is given below (M = 140). Hint: This molecule contains one Si atom.

- a. Propose a molecular formula. $C_3H_6SiCl_2$
 Calculate #C: $(0.6/18.6)/(1.11/98.89) = 2.93$
 M+2 peak is ~60% height of M peak. Must be Cl (2 of them).
 Calculate #Cl: $(12.7/18.6)/(24.23/75.77) = 2.1$

- b. What is the unsaturation number? **1**
- c. Propose a **reasonable** structure for this compound.

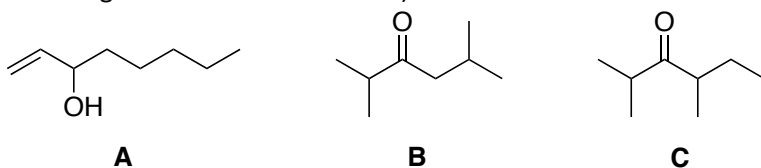


(Or something else reasonable.)



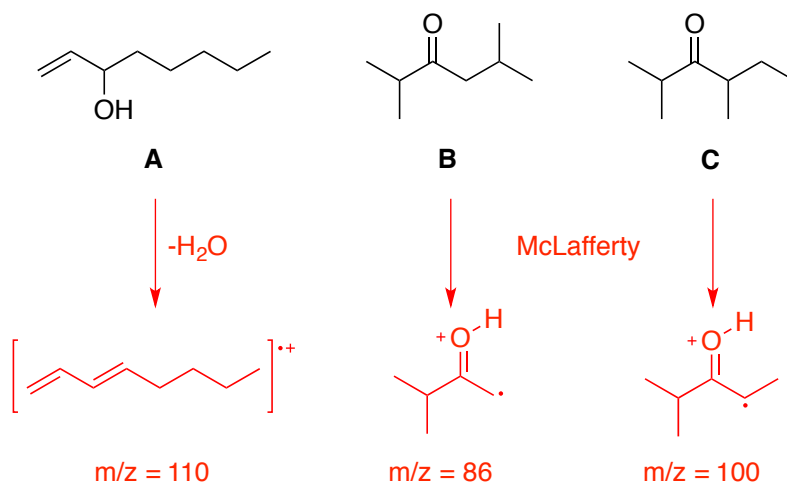
m/z	relative abundance	m/z	relative abundance	m/z	relative abundance	m/z	relative abundance
27.0	2.0	79.0	5.6	107.0	2.7	128.0	5.0
39.0	1.7	80.0	1.5	112.0	5.5	129.0	13.1
42.0	1.0	81.0	1.8	113.0	29.2	140.0 (M)	18.6
43.0	2.2	98.0	4.1	114.0	5.4	141.0	0.6
53.0	2.8	99.0	15.3	115.0	19.5	142.0	12.7
63.0	22.3	100.0	3.6	116.0	1.8	143.0	0.4
64.0	1.7	101.0	10.4	117.0	3.6	144.0	2.5
65.0	8.4	102.0	1.0	125.0	100.0		
77.0	1.7	103.0	2.1	126.0	7.7		
78.0	3.5	105.0	7.5	127.0	69.5		

2. Explain how you would use mass spectrometry to distinguish between the following three isomers (M = 128). Be specific, and draw any important fragment ions that support your answer. (You do not need to draw fragmentation mechanisms.)

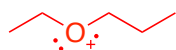


A: Wouldn't expect to see a very large molecular ion peak – dehydration would be especially fast here, because the product is a conjugated diene.

B and C will have different McLafferty fragments, which will be easy to identify as they will be even.

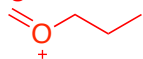


3. Propose the structure of an **ether** (M = 88) with major fragment ions at m/z 73, 59, 43, and 29. Support your answer with clearly drawn mechanisms that lead to these fragment ions.

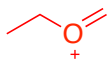


Exact Mass: 88

fragments from α -cleavage:



Exact Mass: 73



Exact Mass: 59

fragments from inductive cleavage:



Exact Mass: 43



Exact Mass: 29

See your notes for mechanisms.

Supplemental data

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%
Fluorine	^{19}F : 100%			
Chlorine	^{35}Cl : 75.77%	^{37}Cl : 24.23%		
Bromine	^{79}Br : 50.69%	^{81}Br : 49.31%		
Iodine	^{127}I : 100%			

1 H 1.00794											1 H 1.00794	2 He 4.002602					
3 Li 6.941	4 Be 9.012182											5 B 10.811	6 C 12.0107	7 N 14.00674	8 O 15.9994	9 F 18.9984032	10 Ne 20.1797
11 Na 22.989770	12 Mg 24.3050											13 Al 26.981538	14 Si 28.0855	15 P 30.973761	16 S 32.066	17 Cl 35.4527	18 Ar 39.948
19 K 39.0983	20 Ca 40.078	21 Sc 44.955910	22 Ti 47.867	23 V 50.9415	24 Cr 51.9961	25 Mn 54.938049	26 Fe 55.845	27 Co 58.933200	28 Ni 58.6934	29 Cu 63.546	30 Zn 65.39	31 Ga 69.723	32 Ge 72.61	33 As 74.92160	34 Se 78.96	35 Br 79.904	36 Kr 83.80