

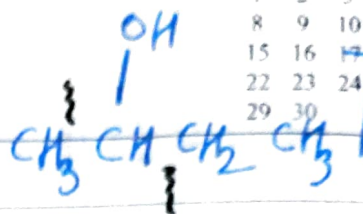
Mass 25

Spectrum
THURSDAY
WEEK 17 • 116-250

of

2-butanol →

APRIL 2024						
M	T	W	T	F	S	S
1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28
29	30					



Relative Abundance

50

20

40

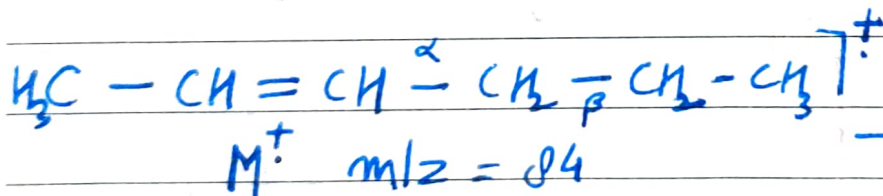
60

80

m/z

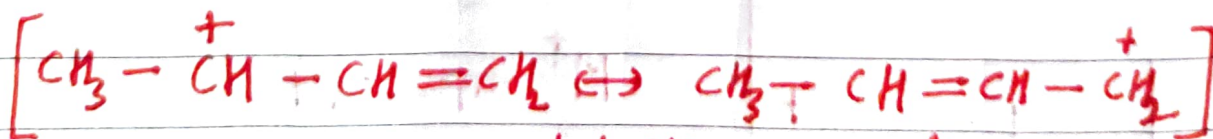
Mass Spectrum of Alkenes →

2-hexene



$m/z = 55$

(base peak) CH_2CH_3



a resonance stabilised allylic cation

MAY							2024						
M	T	W	T	F	S	S	M	T	W	T	F	S	S
			1	2	3	4	5						
6	7	8	9	10	11	12							
13	14	15	16	17	18	19							
20	21	22	23	24	25	26							
27	28	29	30	31									

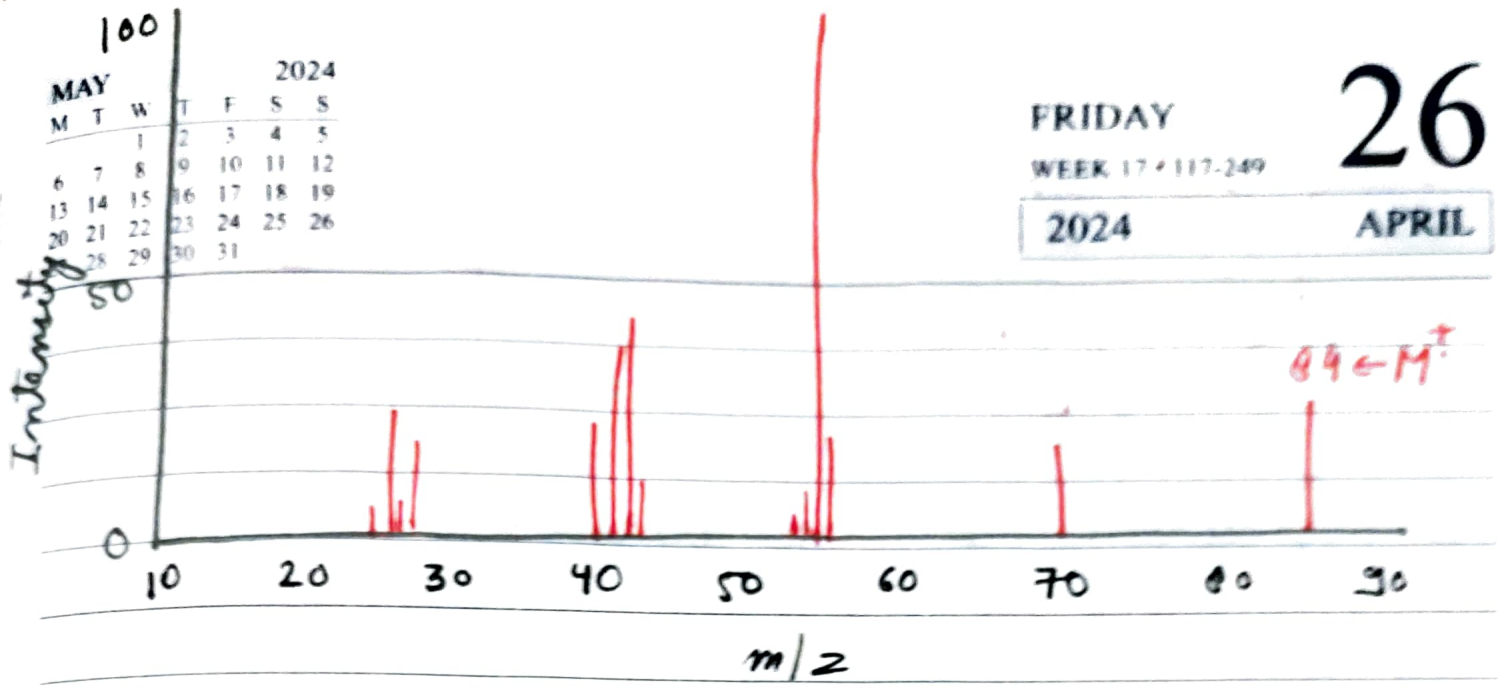
FRIDAY

WEEK 17 • 117-249

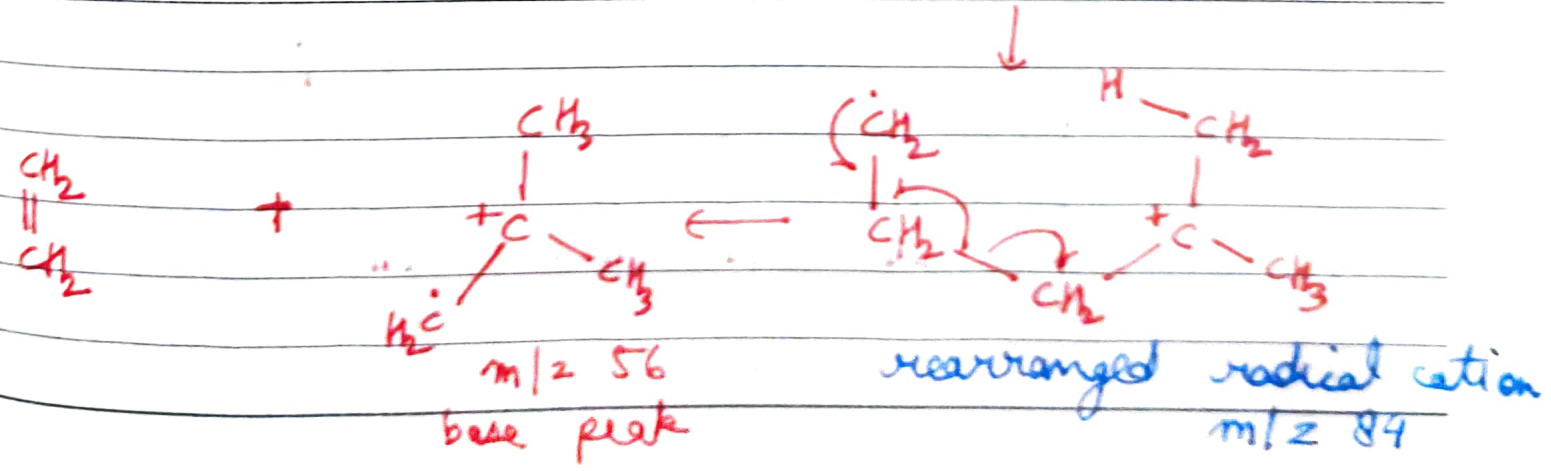
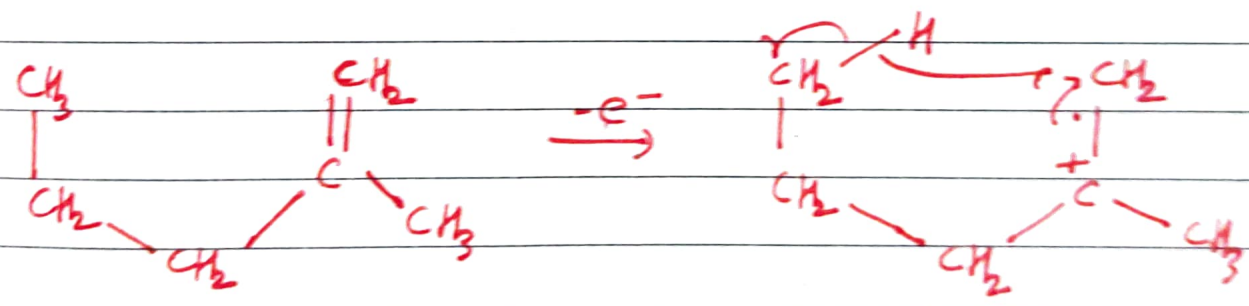
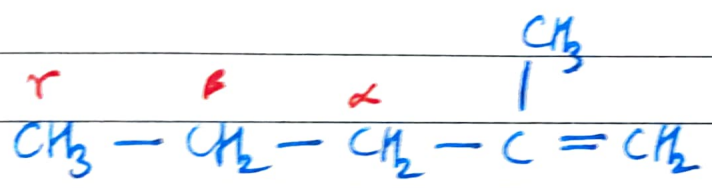
2024

26

APRIL



2-methyl-1-pentene



Similarly,

1-Hexene

27

SATURDAY

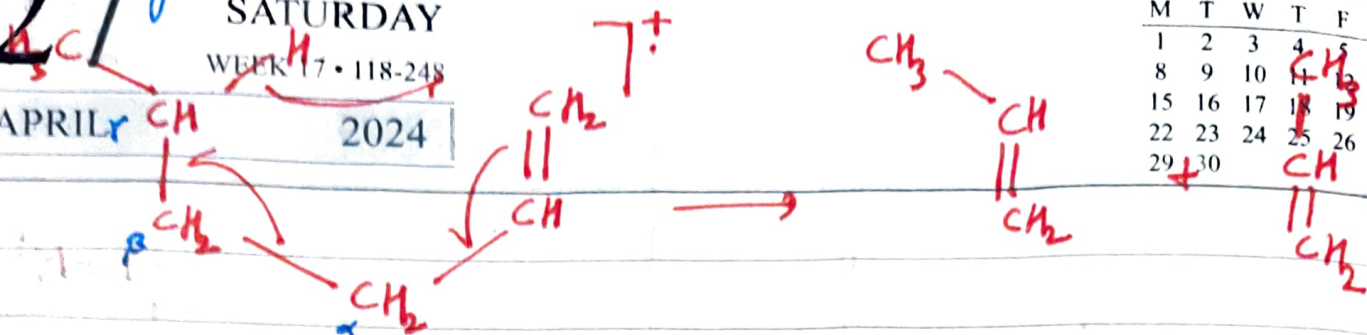
WEEK 17 • 118-248

APRIL

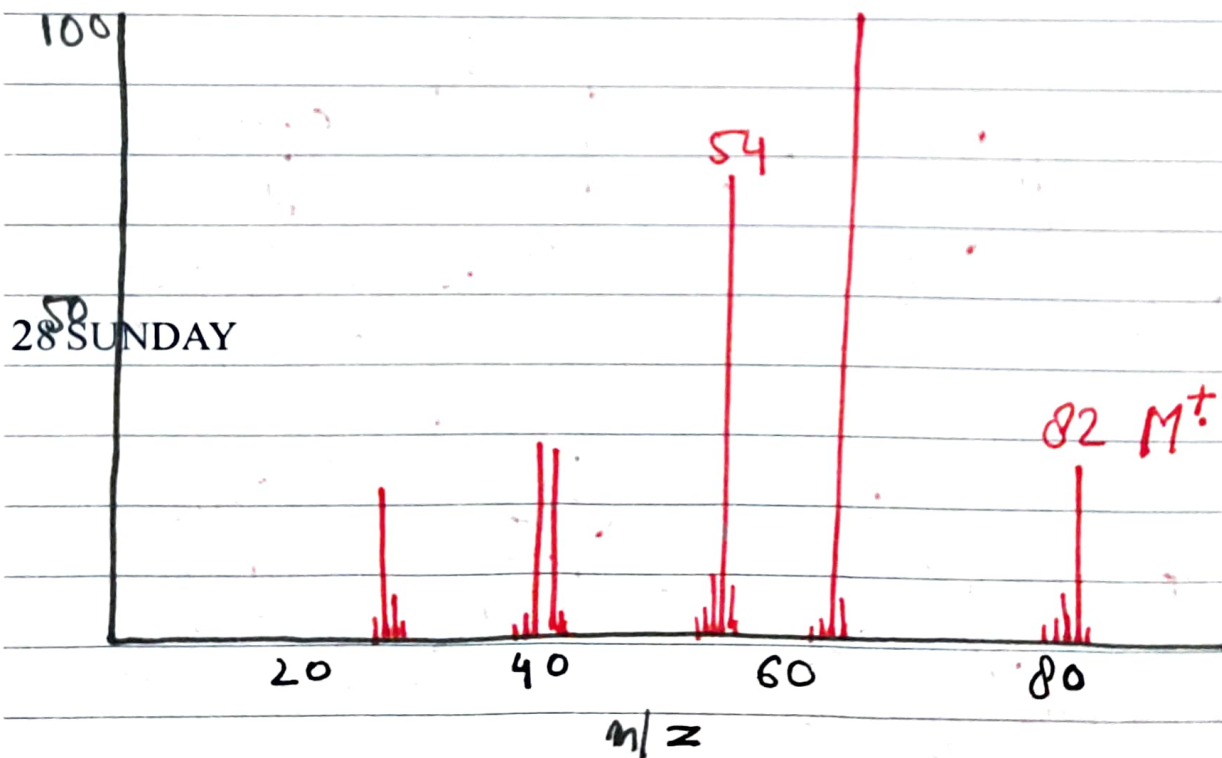
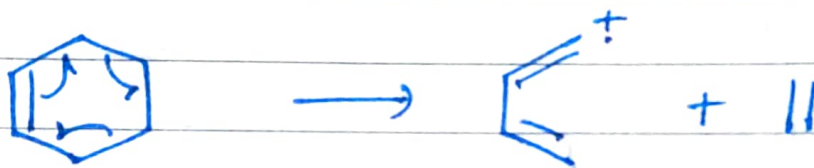
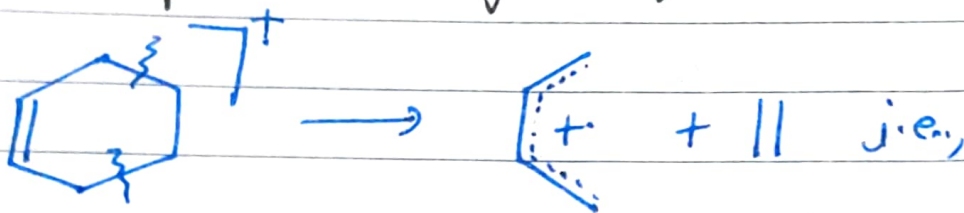
2024

APRIL

M	T	W	T	F	S	S
1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28
29	30					



Mass Spectrum of Cycloalkenes



Relative Abundance

28 SUNDAY

Aromatic Hydrocarbons

2024

MAY						
M	T	W	T	F	S	S
		1	2	3	4	5
6	7	8	9	10	11	12
13	14	15	16	17	18	19
20	21	22	23	24	25	26
27	28	29	30	31		

MONDAY

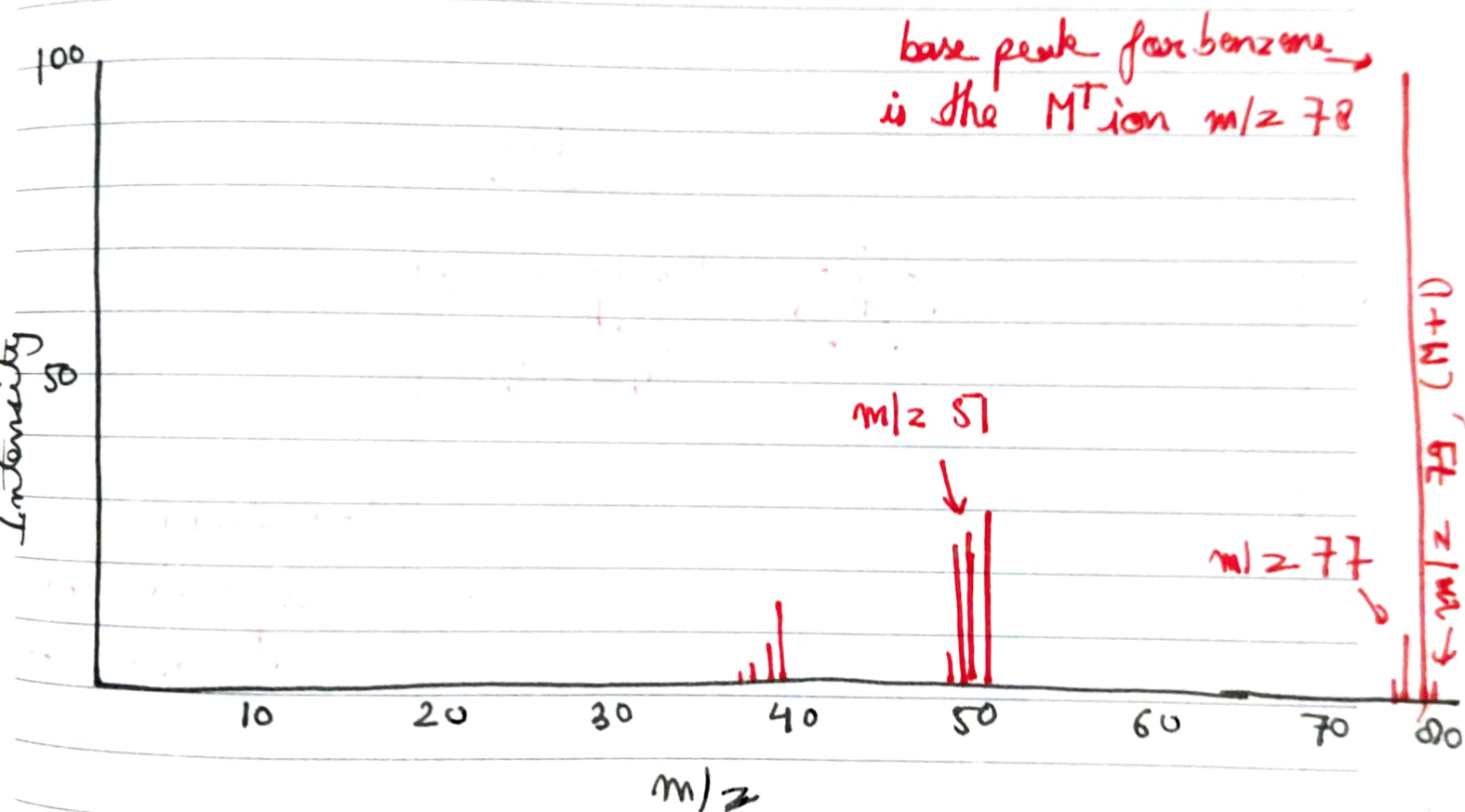
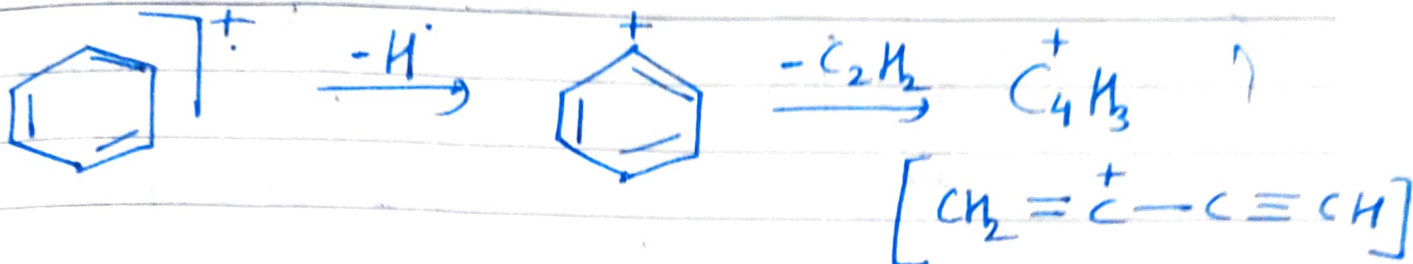
29

WEEK 18 • 120-246

2024

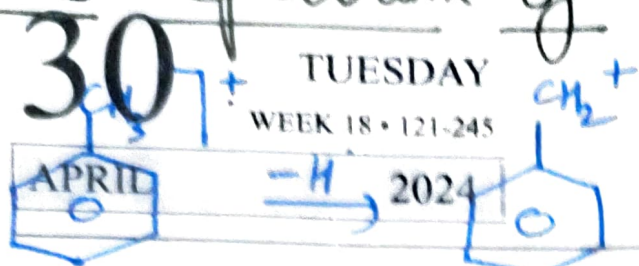
APRIL

Mass Spectrum of Benzene

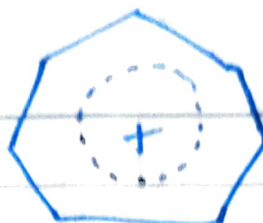


Mass Spectrum of Toluene

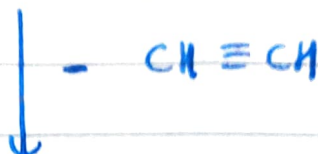
APRIL							2024
M	T	W	T	F	S	S	
1	2	3	4	5	6	7	
8	9	10	11	12	13	14	
15	16	17	18	19	20	21	
22	23	24	25	26	27	28	



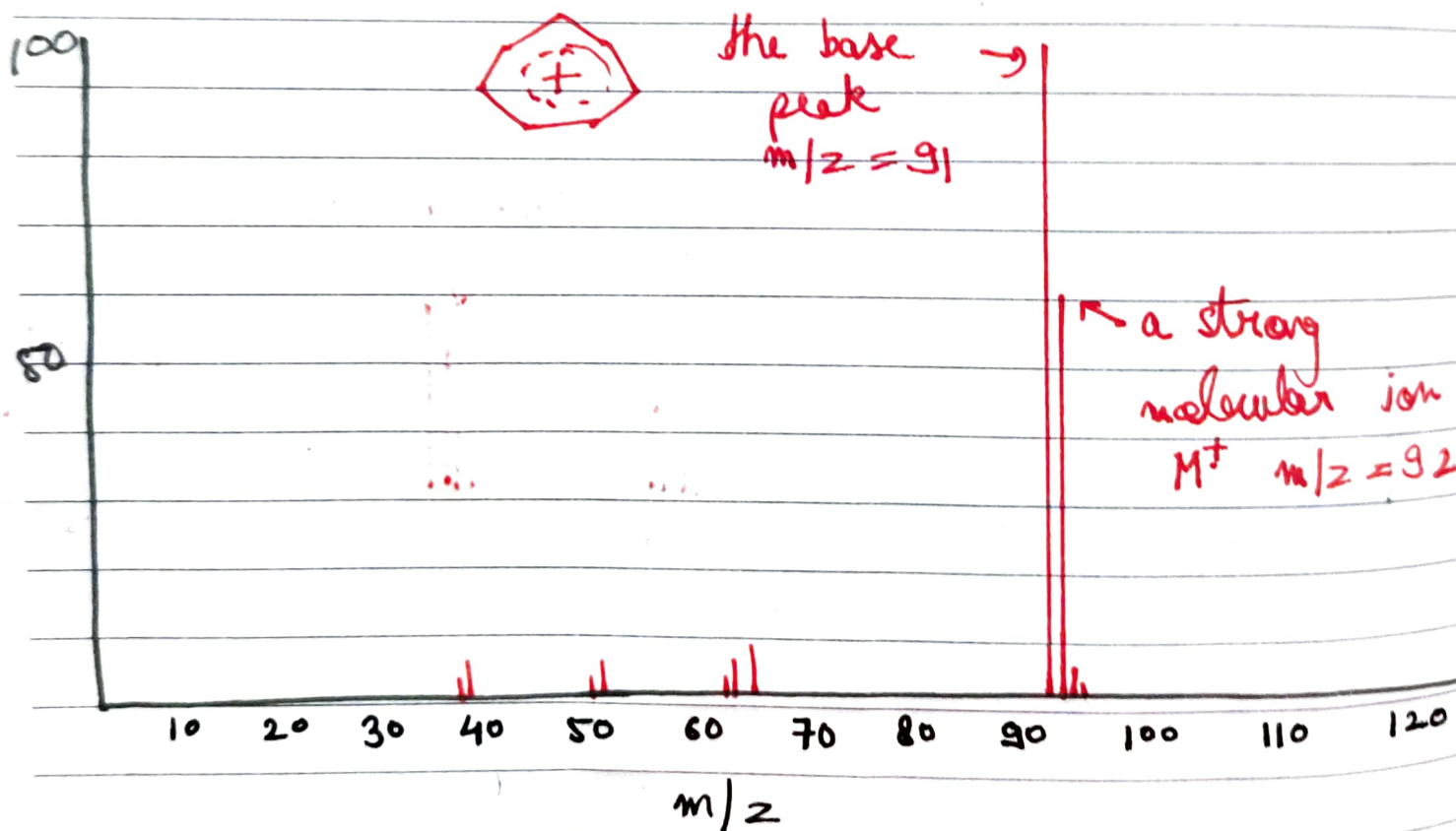
benzyl cation



tropylium cation



Relative Abundance



Hydroxy Compounds

MAY 2024
 W T F S S
 1 2 3 4 5 6 7 8 9 10 11 12
 13 14 15 16 17 18 19
 20 21 22 23 24 25 26
 27 28 29 30 31
Alcohol

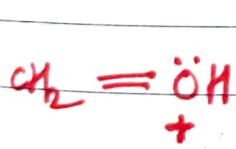
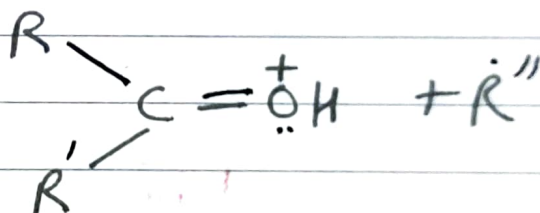
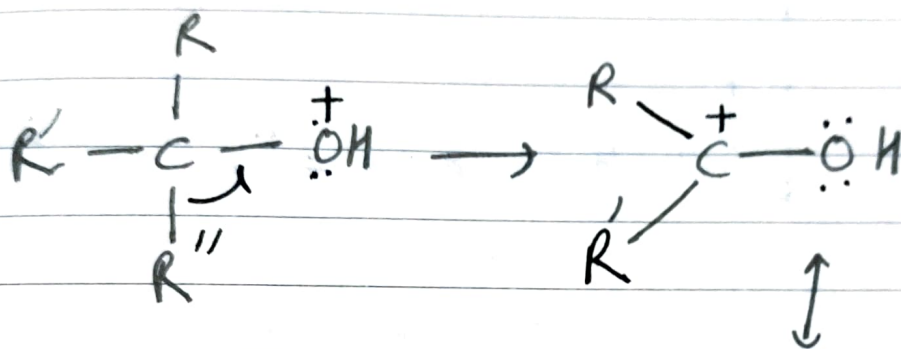
WEDNESDAY
 WEEK 18 • 122-244

01

2024

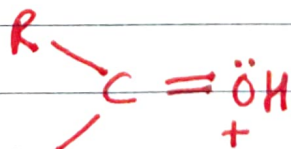
MAY

Primary and Secondary alcohols usually give weak M^+ ions and for tert. alcohols the M^+ ions is either weak or absent.



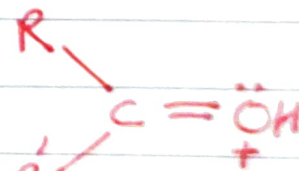
primary

(m/z 31)



secondary

(m/z 45, 59, 73 etc.)



tertiary

(m/z 59, 73, 87, etc.)

Fragmentation of 2-hexenal

02

THURSDAY

WEEK 18 • 123-243

MAY

MAY 2 2024



$m/z = 102$

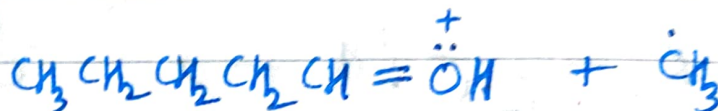
M^+

2-hexenal

α -cleavage



loss of largest alkyl group is preferred pathway



$m/z = 87$

a smaller peak at

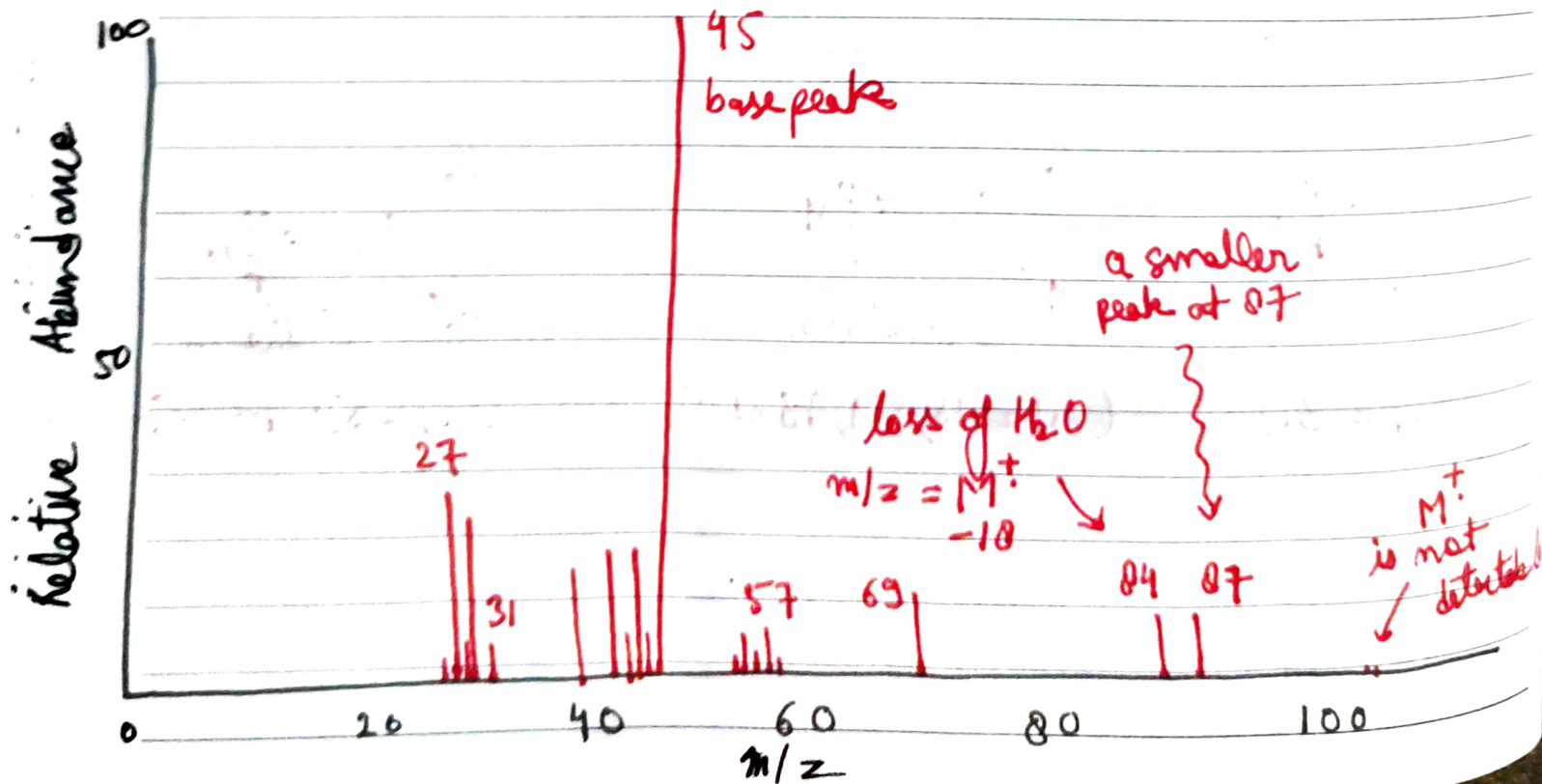
$m/z = 87$

(α -cleavage of methyl group)

MAY

M	T	W	T	F	S	S
6	7	8	9	10	11	12
13	14	15	16	17	18	19
20	21	22	23	24	25	26
27	28	29	30	31		

(base peak)



Fragmentation of 1-butanol →

JUNE							2024	
M	T	W	T	F	S	S		
					1	2		
3	4	5	6	7	8	9		
10	11	12	13	14	15	16		
17	18	19	20	21	22	23		
24	25	26	27	28	29	30		

FRIDAY

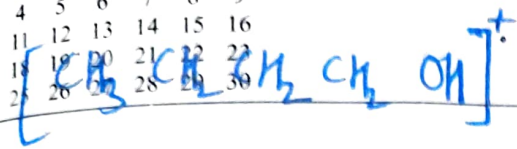
WEEK 124-242

2024

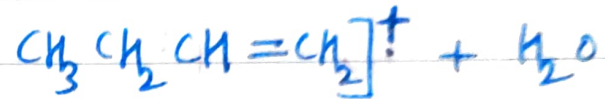
03

MAY

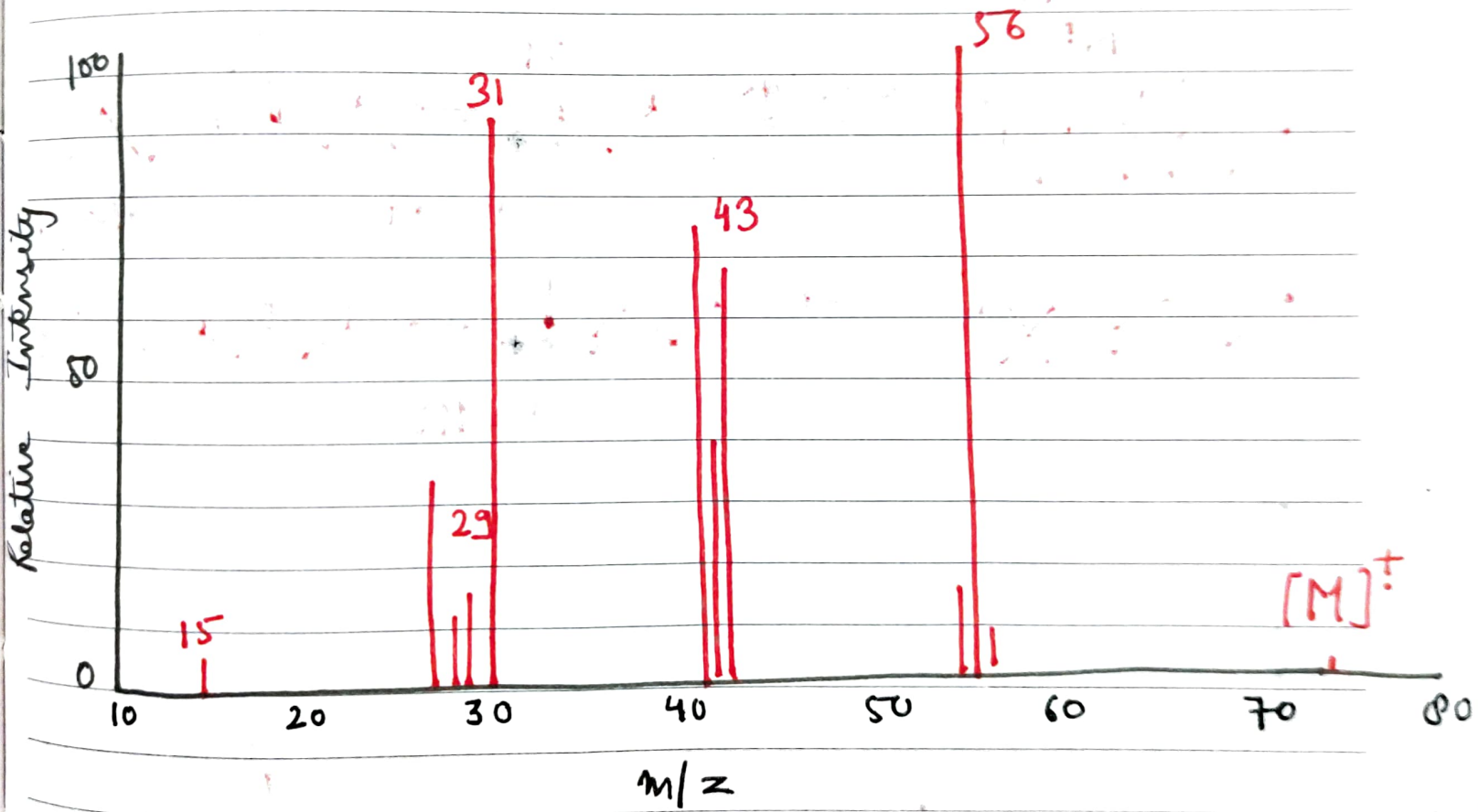
m/z 31



α-cleavage



m/z = 56



Fragmentation of 2,6-dimethyl-4-heptanol

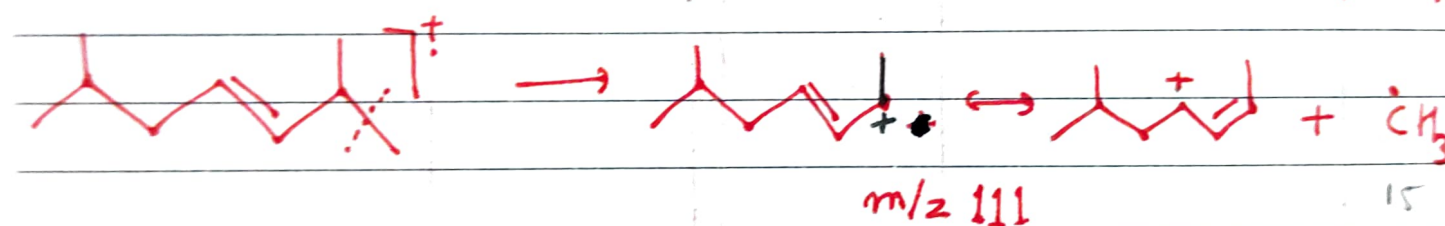
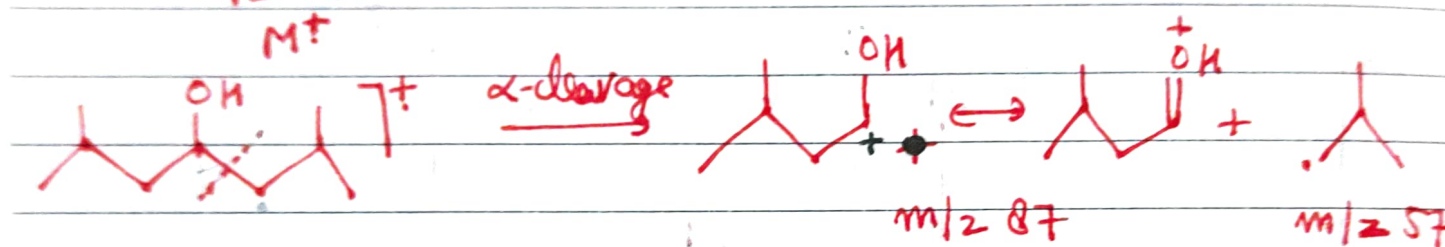
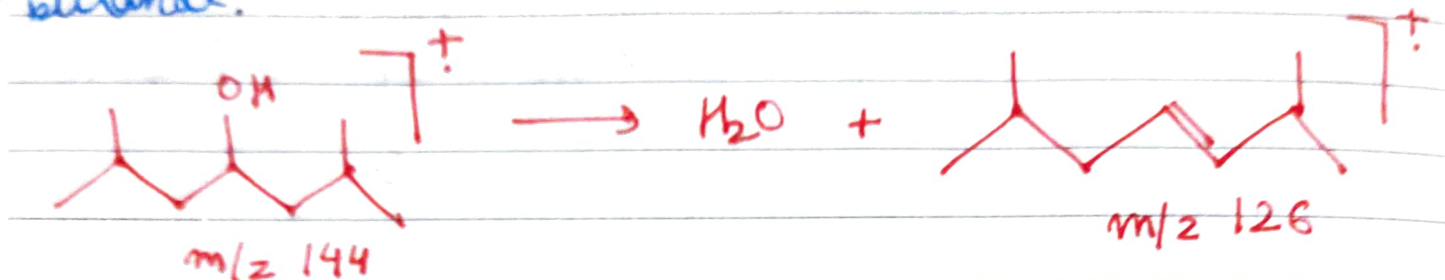
04

SATURDAY

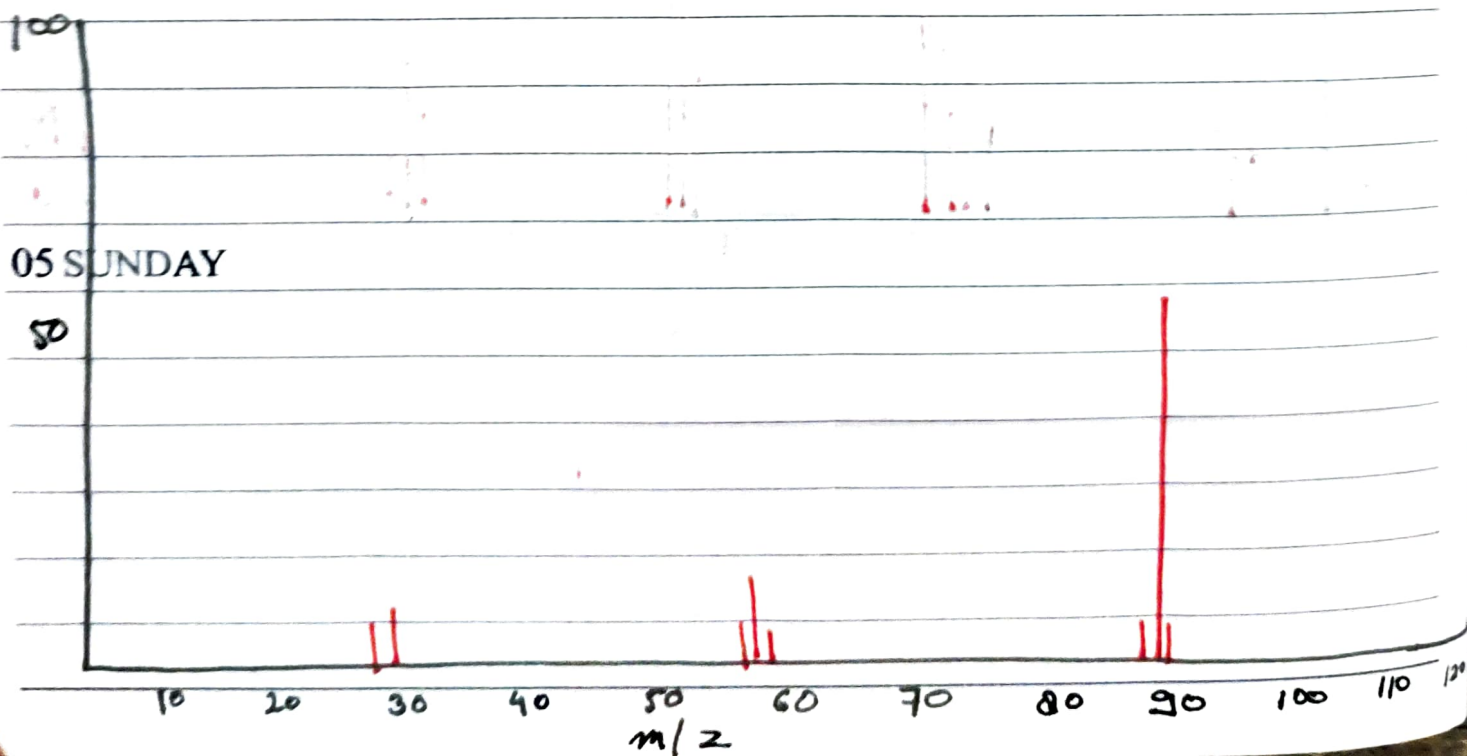
MAY 04 2024
The fragmentation of 2,6-dimethyl-4-heptanol (mol. mass 144) is similar to that of 1-butanol.

MAY 2024						
M	T	W	T	F	S	S
					4	5
6	7	8	9	10	11	12
13	14	15	16	17	18	19
20	21	22	23	24	25	26
27	28	29	30	31		

1-butanol.



Relative Intensity



Fragmentation of Cyclic Alcohols →

2024

JUNE						
M	T	W	T	F	S	S
				1	2	
3	4	5	6	7	8	9
10	11	12	13	14	15	16
17	18	19	20	21	22	23
24	25	26	27	28	29	30

spectra of cyclic alcohols

MONDAY

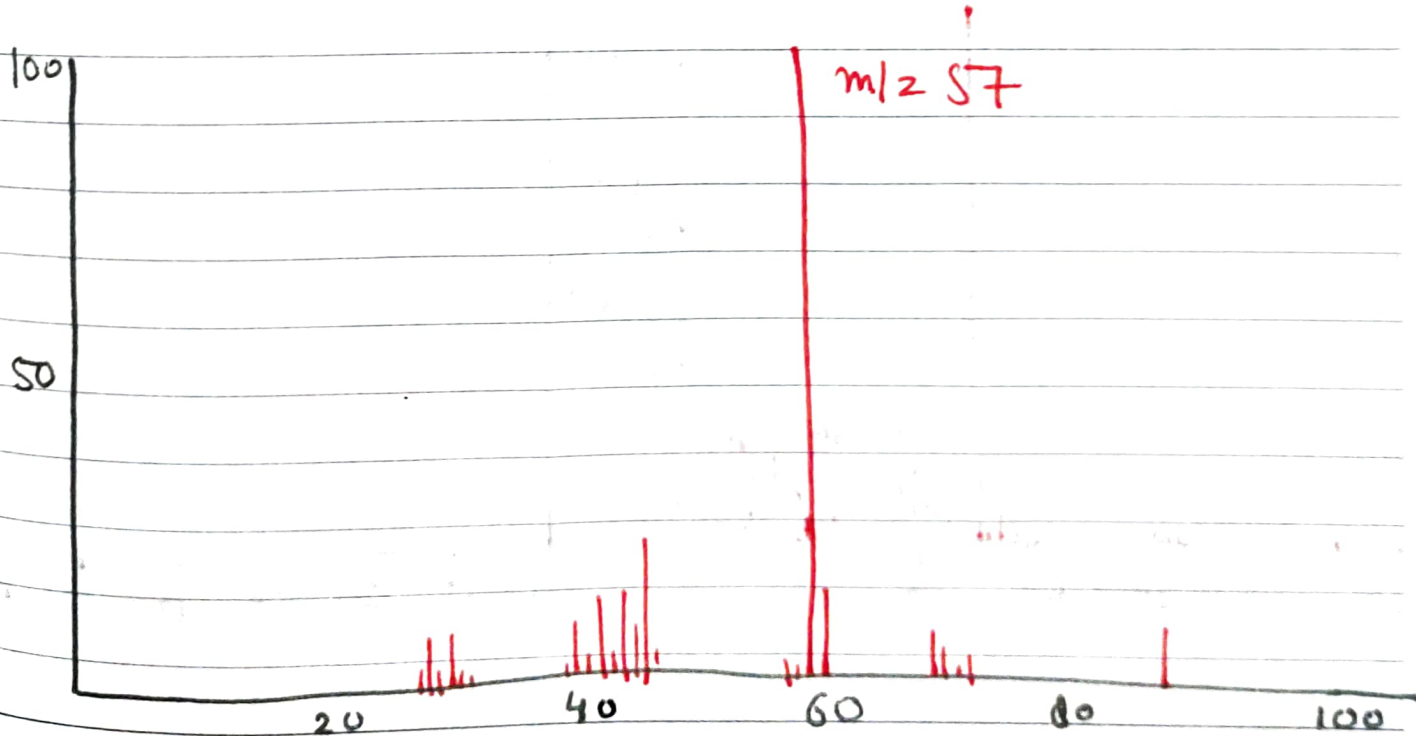
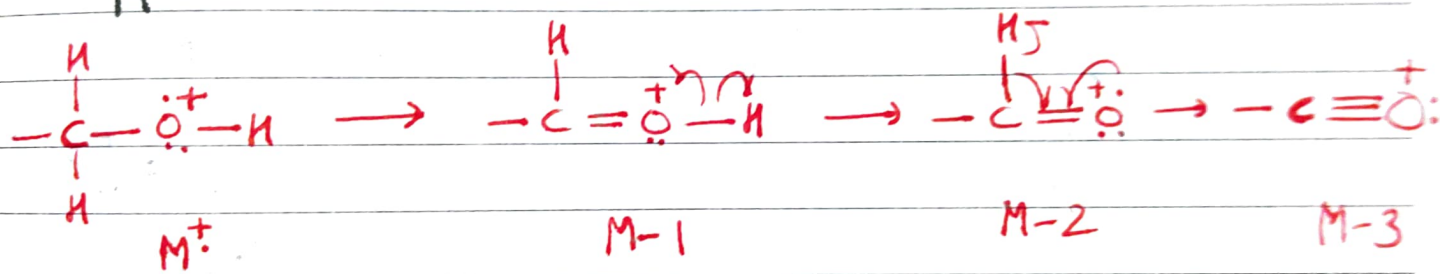
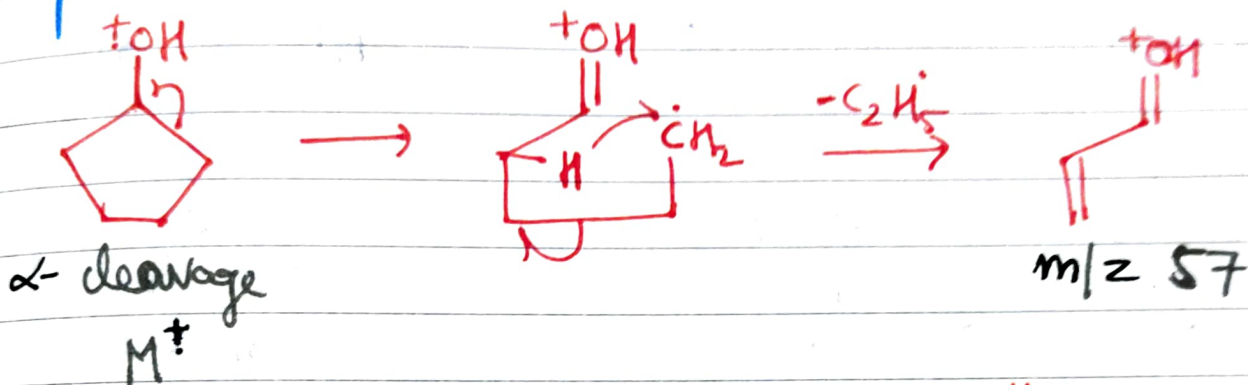
2-06

WEEK 19 • 127-239

2024

MAY

results in ring opening which followed by unexpected but easily rationalised processes.



Molecular Weight and Formula Determination

2024

JUNE

M	T	W	T	F	S	S
		1	2	3	4	5
6	7	8	9	10	11	12
13	14	15	16	17	18	19
20	21	22	23	24	25	26
27	28	29	30			

WEDNESDAY

WEEK 19

2024

MAY

08

Consider a molecular ion peak at m/z at 50.

Magic figure 13 (CH) (Remember)

$$\frac{M^+}{13} = \frac{50}{13}$$

$$\begin{array}{r} 13 \overline{) 50} \quad 4 \rightarrow n \\ \underline{52} \\ 6 \rightarrow r \end{array}$$

Base formula = $C_n H_{n+r}$

$$= C_4 H_{4+6}$$

$$= \underline{C_4 H_{10}} \text{ molecular ion}$$

Common Fragment Ions

m/z 99
MAY

THURSDAY
WEEK 19 • 130-236

2024

Ion

Possible

MAY							2024
M	T	W	T	F	S	S	
			1	2	3	4	5
6	7	8	9	10	11	12	
13	14	15	16	17	18	19	
20	21	22	23	24	25	26	
27	28	29	30	31			

31 $\text{CH}_2 = \text{OH}^+$ 1° alcohol

30 $\text{CH}_2 = \text{NH}_2^+$ 1° amine

43 C_3H_7^+ alkane

45 $\text{CH}_3\text{CH} = \text{OH}^+$ 2° alcohol

59 $\text{CH}_3 - \underset{\text{CH}_3}{\text{C}} = \text{OH}^+$ 3° alcohol

91 C_7H_7^+ $\text{C}_6\text{H}_5 - \text{CH}_2\text{R}$

Q. Consider a compound forms peaks at values of 100, 85, 71, 57, 43 (100%)
 molecular formula

JUNE 2024						
M	T	W	T	F	S	S
					1	2
3	4	5	6	7	8	9
10	11	12	13	14	15	16
17	18	19	20	21	22	23
24	25	26	27	28	29	30

FRIDAY, 71, 57, 100 (100%)
 WEEK 19 • 131-235

2024

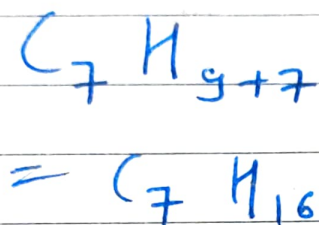
MAY

Soln

$$M^+ = 100$$

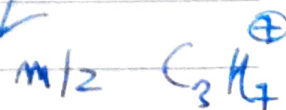
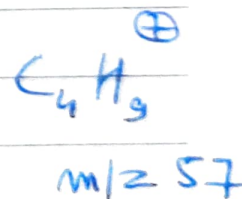
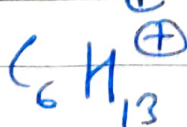
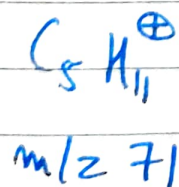
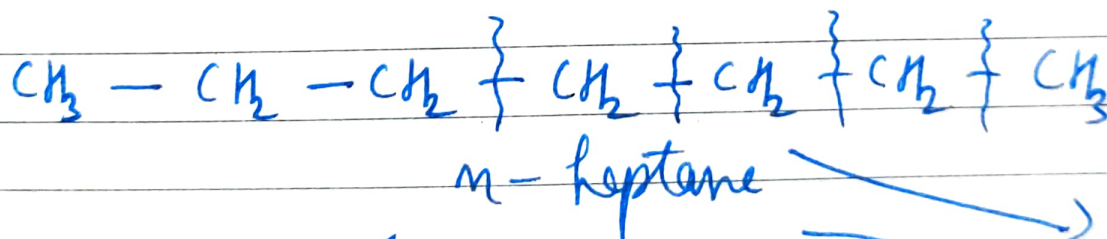
$$\frac{M^+}{13} = \frac{100}{13}$$

$$\begin{array}{r} 7 \rightarrow n \\ 13 \overline{) 100} \\ \underline{91} \\ 9 \rightarrow n \end{array}$$



$$\begin{array}{r} 57 \\ - 43 \\ \hline 14 \end{array}$$

Here difference is of 14
 alkanes $\rightarrow$ 14 unit apart



93