65.3201* P.S #2

Chapt 8 #1 : $C_{43}H_{50}N_4O_6$

Using most abundant isotopes : calc'd "precise mass"

$= 43(12.00000) + 50(1.00783) + 4(14.0031)$

$+ 6(15.9949)$

$= 718.3733$

$C_{42}H_{46}N_4O_7$: calc'd "precise mass"

$= 42(12.0000) + 46(1.00783) + 4(14.0031)$

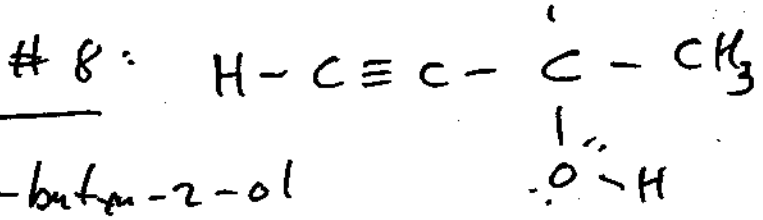
$+ 7(15.9949)$

$= 718.33688$

Since the obs'd "precise mass" is 718.3743

$C_{43}H_{50}N_4O_6$ is a much better fit!

Chapt 8 #8:



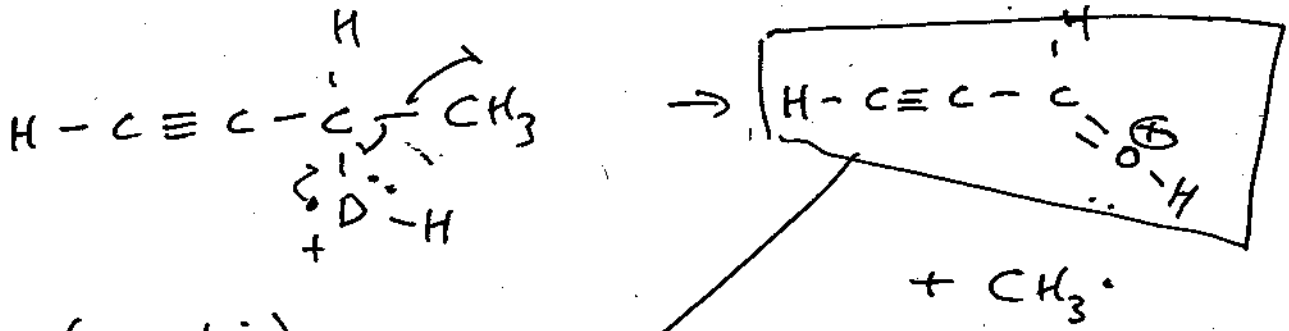
3-butyn-2-ol

Parent (molecular ion) expected at

m/e = 70 for C_4H_6O

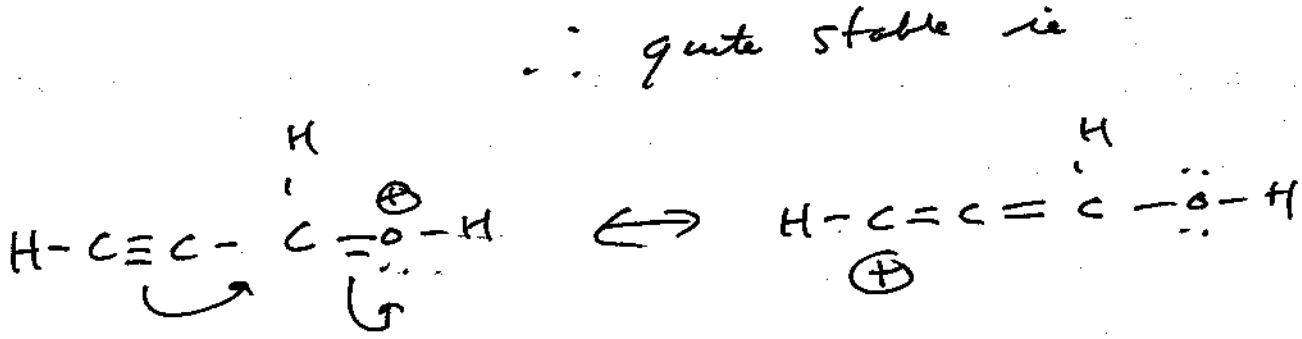
∴ m/e = 55 probably comes from loss of a CH_3 group.

Possible mechanism:



(parent ion)
a radical ion

can be stabilized by resonance.
∴ quite stable ie



Chapt 8 #10. (e) IR looks like NH or NH_2 (3280 cm^{-1})

also add molecular weight suggests N is present

Chapt 8 # 10 (e) cont'd

Using the "rule of 13"

Base formula: $\frac{129}{13} = n + {}^{r}/_{13}$

$= 9 + 12$

∴ "Base formula" = C_9H_{21}

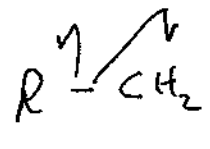
But, N is present, ∴ need to subtract CH_2 and add N

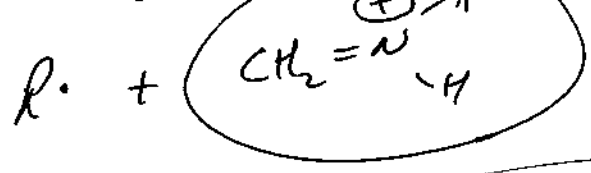
∴ Molecular formula could be $C_8H_{19}N$

$(96 + 19 + 14) = 129$

units of unsat'n $= 9 - \frac{19}{2} + \frac{1}{2} = 0$

Looking at fragmentation pattern: peak at m/e = 30 suggests $R-CH_2-NH_2$

arises via: 

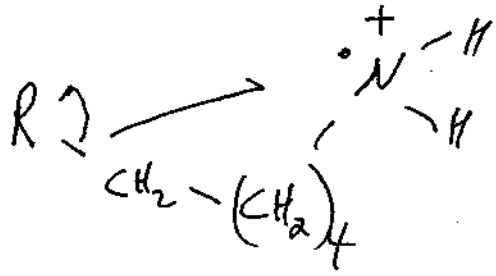
(Pavia, p 430) 

m/e = 30

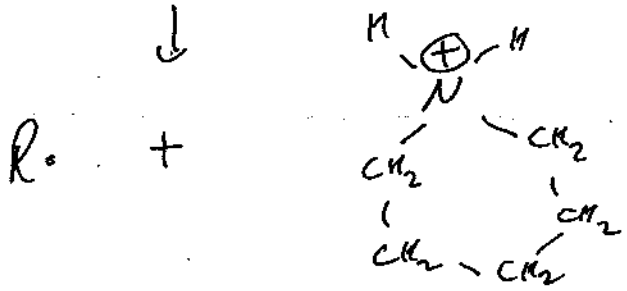
origin of m/e 86: (see Pavia p 435):

But, ✗ Incorrect Arrow Pushing!

(D)



(6-m'd ring formed, ∴ favored!)



$C_5H_{12}N$

m/e = 86

So a possible structure is $CH_3(CH_2)_7-NH_2$

or