^{13}C isotope usage

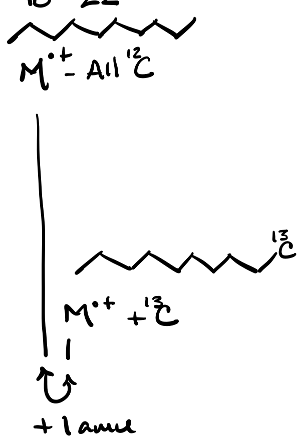
^{12}C vs. ^{13}C

98.9% 1.1%

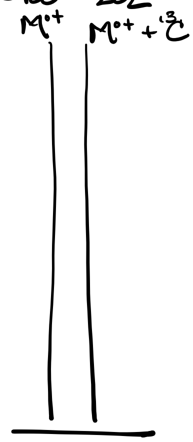
Natural Abundance

$$\frac{^{13}C}{^{12}C + {}^{13}C} \times 100 = 1.1\%$$

$C_{10}H_{22}$



$C_{100}H_{202}$



$10 \times 1.1\% =$ Relab 10

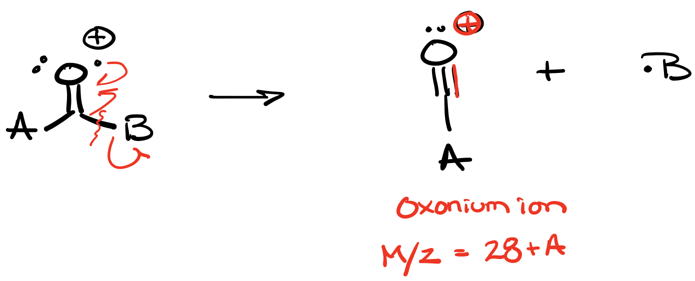
$100 \times 1.1\% =$ Rel Ab 100

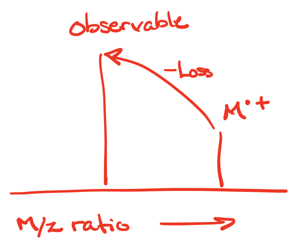
Back Calculation

$$\frac{\left[\frac{(M^{\bullet +} - {}^{13}C)_{Rel\,Ab}}{(M^{\bullet +})_{Rel\,Ab}} \times 100\right]}{1.1} = \#\ \text{Carbons in formula}$$

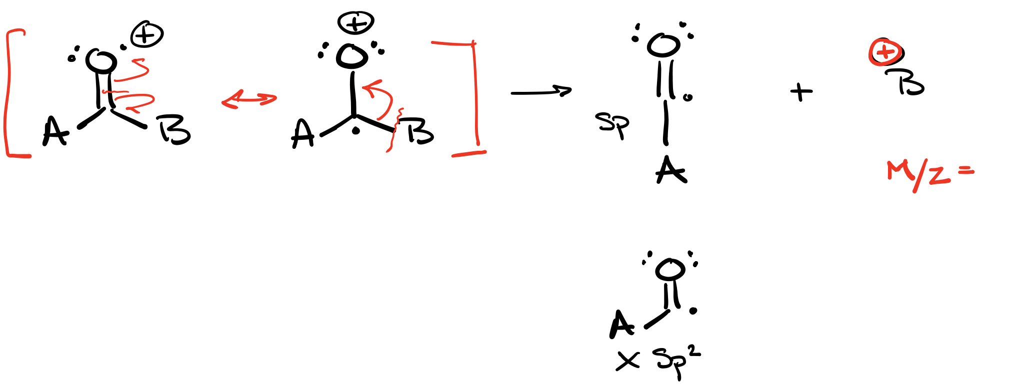
$$\frac{\dfrac{(M^{\bullet +} - {}^{13}C)_{Rel\,Ab}}{(M^{\bullet +})_{Rel\,Ab}} \times 100}{\dfrac{{}^{13}C}{{}^{12}C + {}^{13}C} \times 100} = \#\ \text{Carbons in molecule}$$

#2 Homolytic α - cleavage (Always two possibilities)

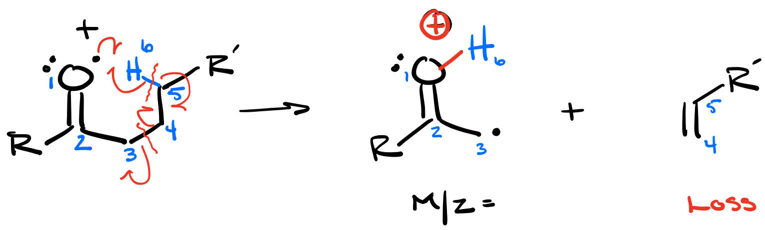


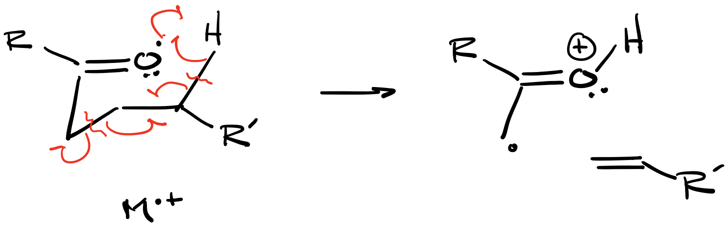


Heterolytic α - Cleavage (Always two possibilities)

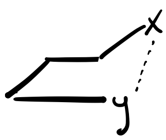


McLafferty Rearrangement



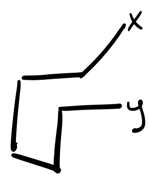


5 ring ‡
Less Common

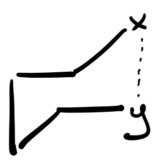


~109.5

7 ring ‡
Less Common



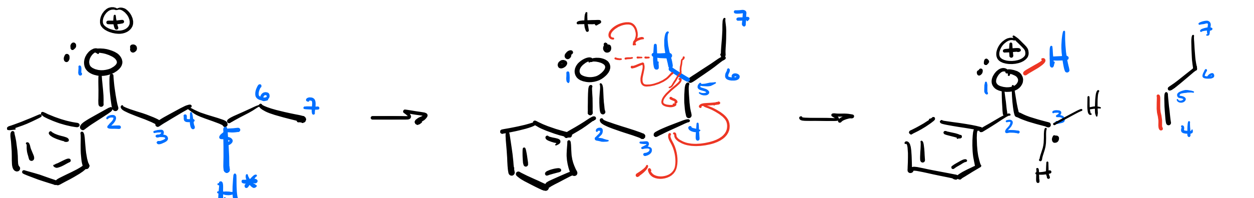
* 6 ring ‡



~ 109.5

Most Common

Examples



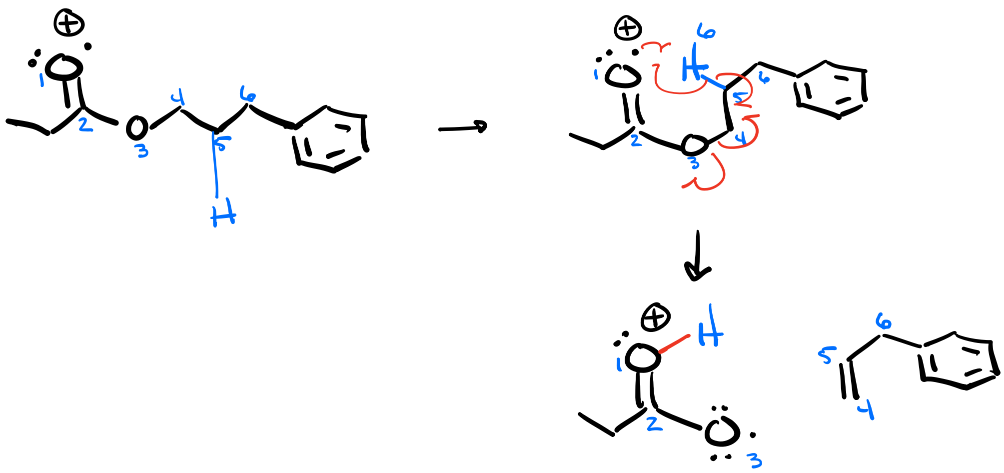
Radical on # 3

$C_8H_8O^{+}$

m/z = 110

Double Bond between 4 & 5

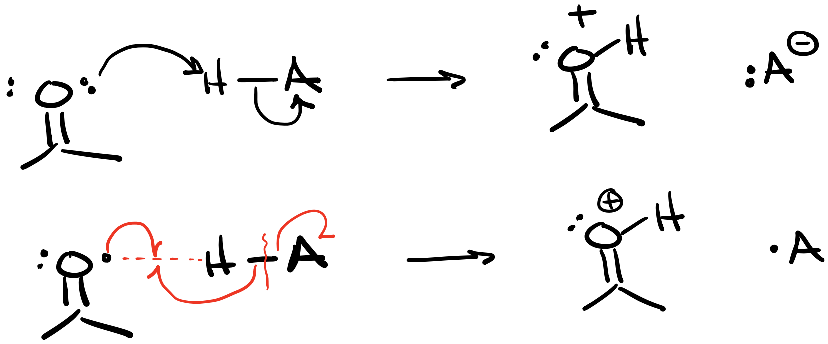
Loss



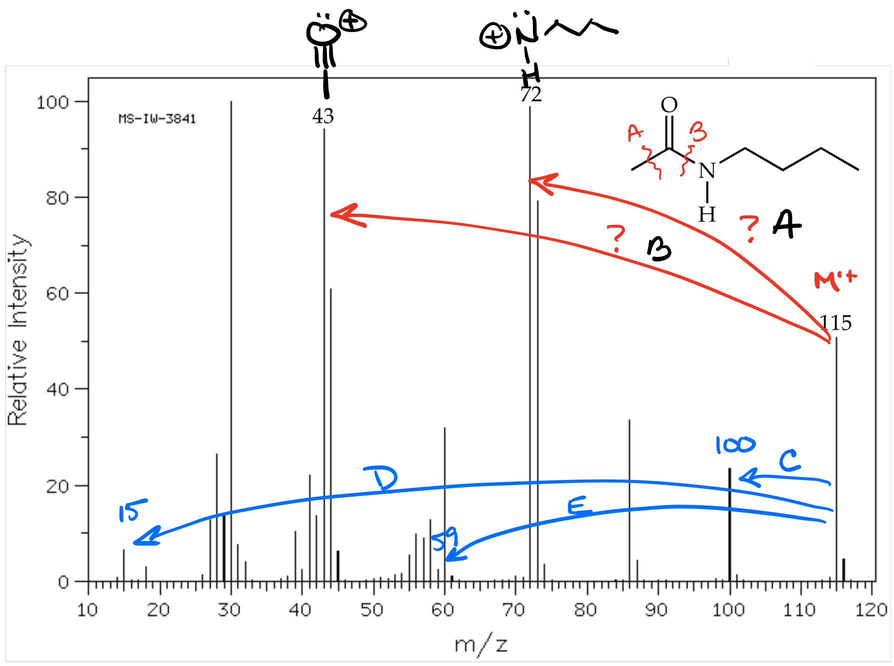
Loss

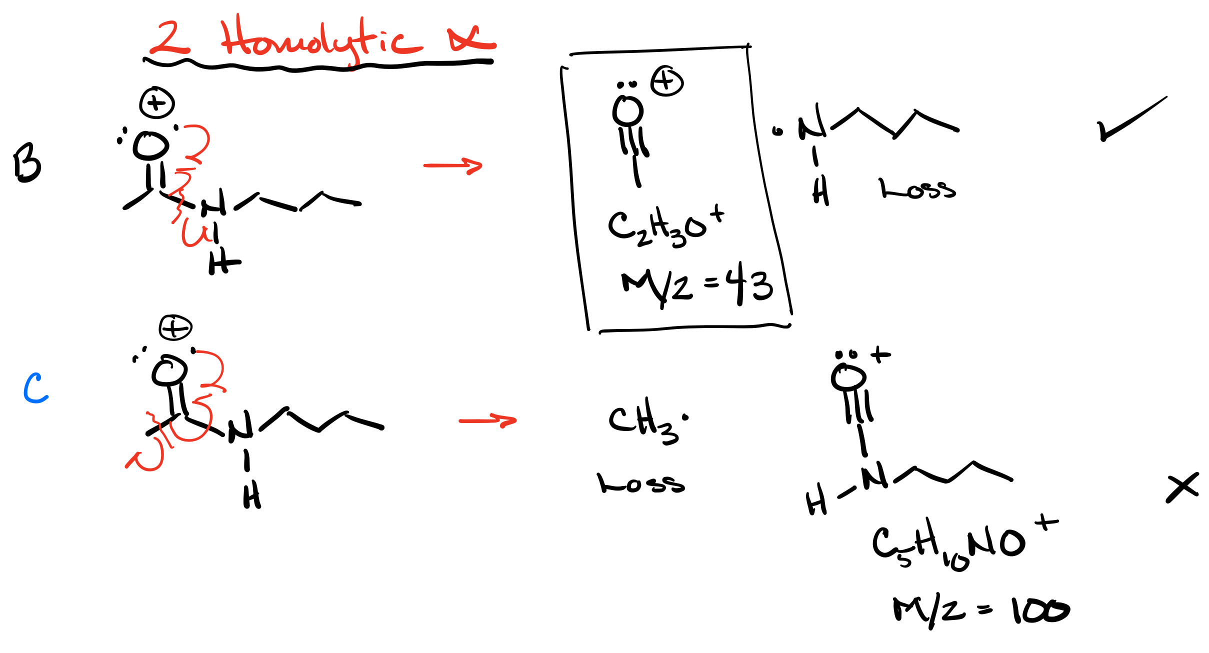
$C_3H_6O_2^{\bullet +}$

m/z = 74



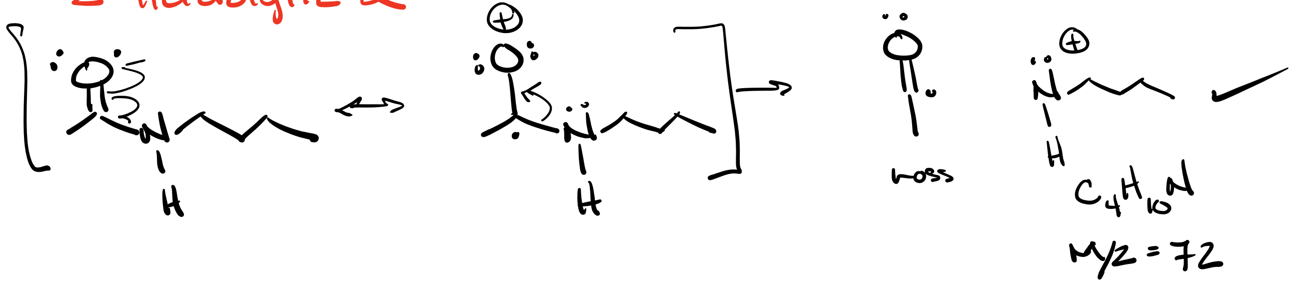
4. [/10] The mass spectrum of *N*-butylacetamide is shown below. Show the mechanisms of the cleavage reactions from the molecular ion that lead to the m/z 72 peak and the m/z 43 peak. You need only consider the homolytic and heterolytic α-cleavages and, if applicable, McLaffertry.



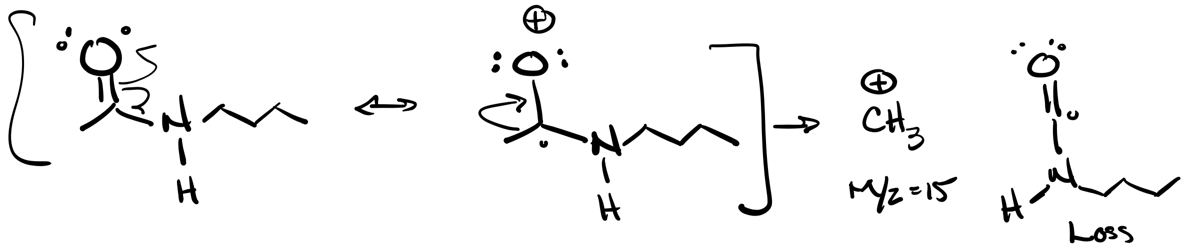


2 Heterolytic α

A

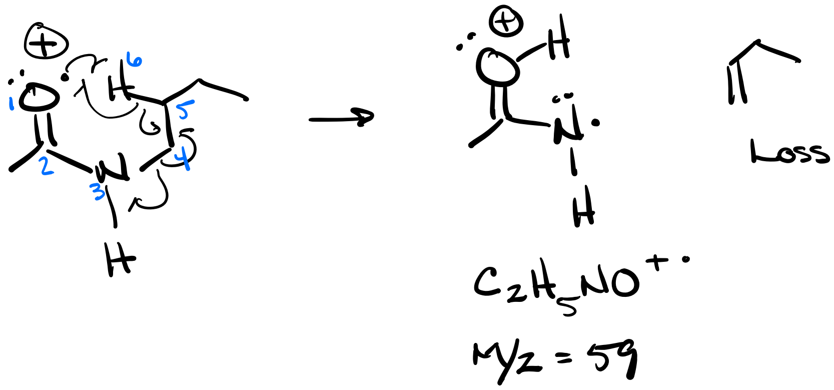


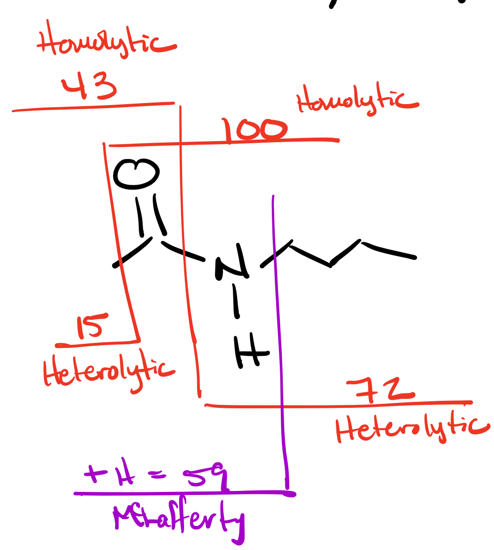
D

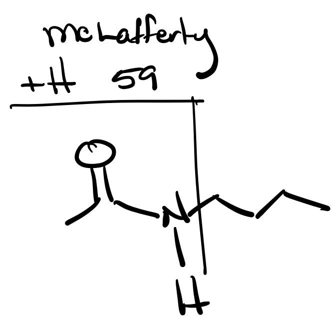


McLafferty

E







MS-MS