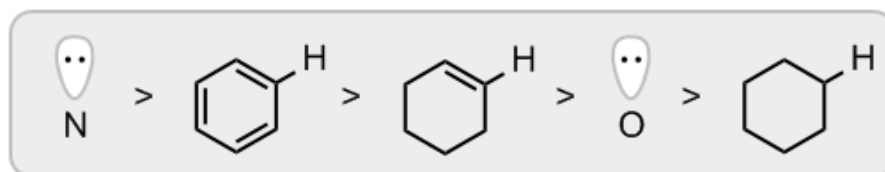


## CONCEPT: MASS SPECT- FRAGMENTATION

### Ionization Potentials:

Some electrons require less energy to ionize than others.

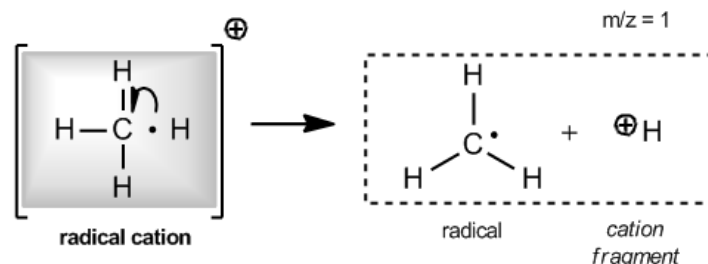
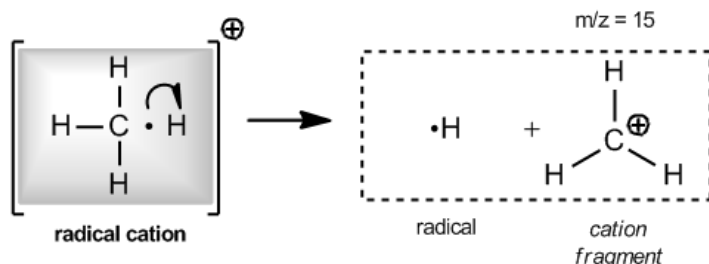
#### Ease of Ionization



### Simple Fragmentation Mechanisms:

The molecular ion will often fragment into smaller, sometimes more stable ion fragments.

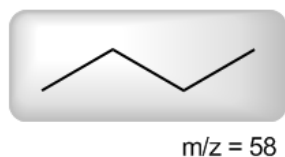
- The stability of the **cation fragment** usually determines the relative amounts of fragments observed
- Radicals tend to form on the *less stable* side of the fragment



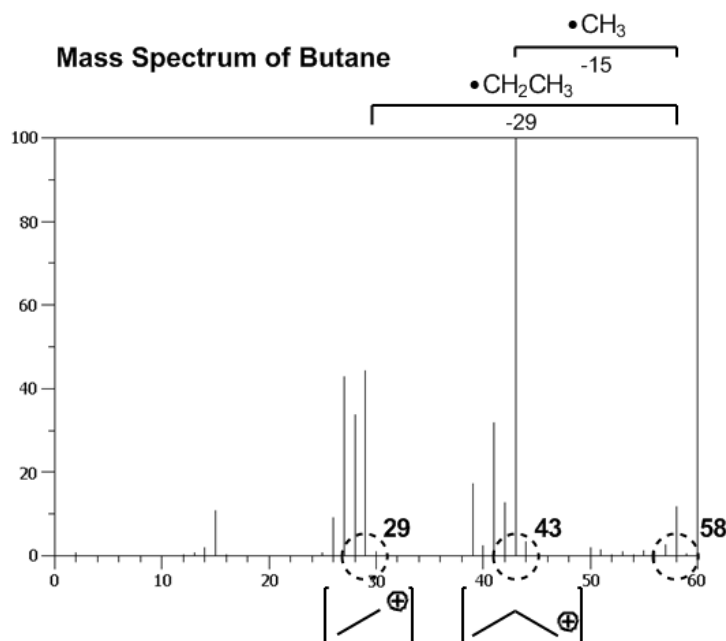
### Common Splitting Fragments:

$M^+ - 15 = \bullet\text{CH}_3$	$M^+ - 31 = \bullet\text{OCH}_3$
$M^+ - 17 = \bullet\text{OH}$	$M^+ - 35 = \bullet\text{Cl}$
$M^+ - 18 = \text{H}_2\text{O}$	$M^+ - 45 = \bullet\text{OCH}_2\text{CH}_3$
$M^+ - 29 = \bullet\text{CH}_2\text{CH}_3$	$M^+ - 80 = \bullet\text{Br}$

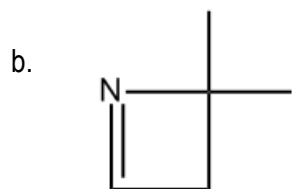
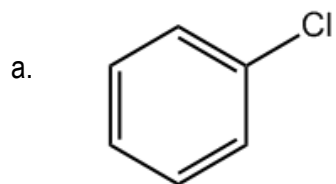
### EXAMPLE: Fragmentation of Butane



electron  
beam



**PRACTICE:** Draw the most likely ion fragment for the following molecules



**PRACTICE:** Propose the molecular ion and likely fragmentation mechanism for the following molecule. What would be the value of the base peak?

