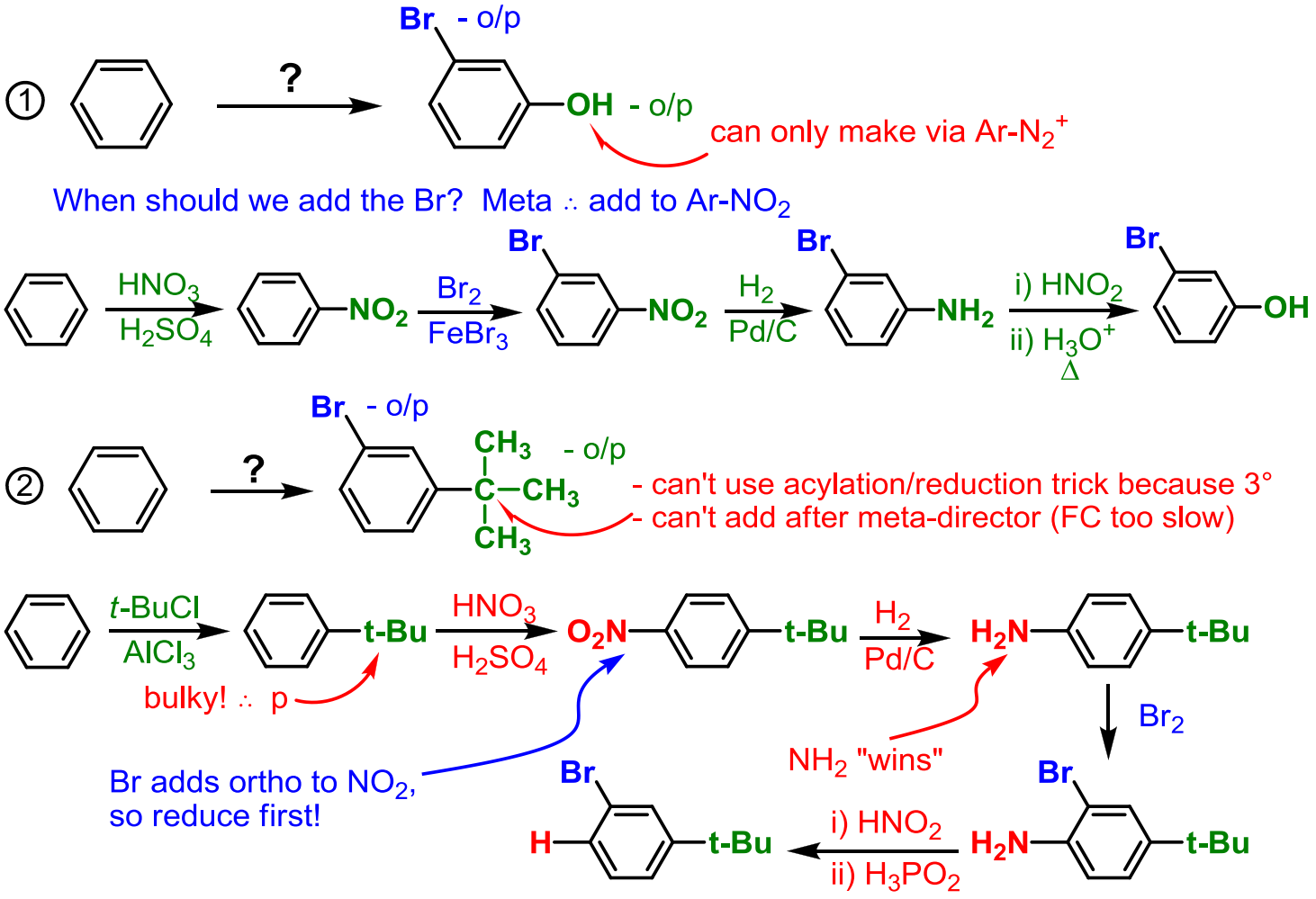
CHEM 242 – Lecture 20 *03/03/2014*

Overheads: - Outline
- Bruice MS & IR overheads

Handout: Aromatics

Recap Friday: Reactions of Substituents on Aromatics - See Handout

Synthesis Examples:



Determining Structure of Organic Molecules: -how do we know what we have?

Main tool is Spectroscopy / Spectrometry

Interaction of matter with light

Interaction of matter with energy (more general)

Three main types:

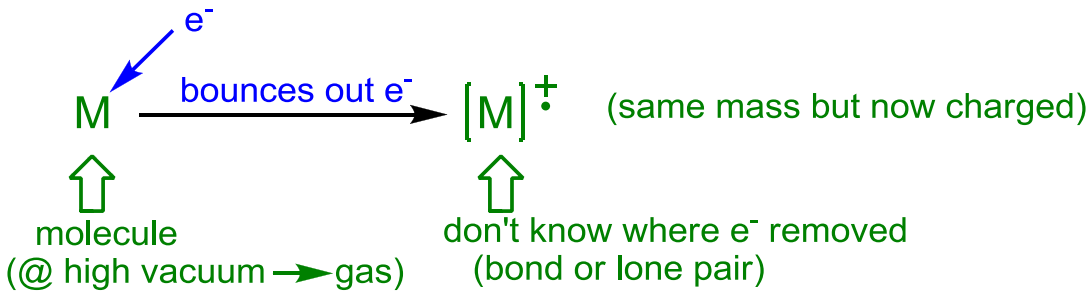
Mass Spectrometry (MS): Gives molecular weight - uses electrons as energy source

Infrared Spectroscopy (IR): Gives functional group info – uses infrared radiation (heat!)

Nuclear Magnetic Resonance Spectroscopy (NMR): Gives most structural info – uses radio waves

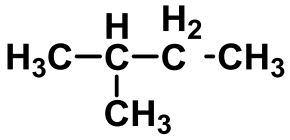
Also UV/Vis: Gives info about conjugated double bonds – uses ultraviolet/visible light

Mass Spectrometry (MS):

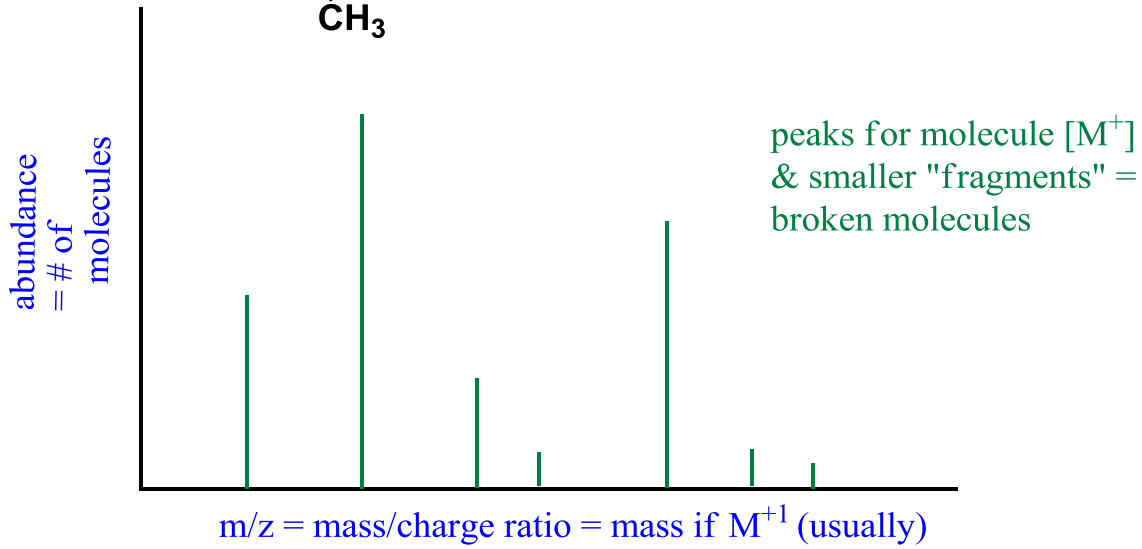


*** Only see cations in mass spec – neutral molecules "pumped off"

Figure 14.1/13.1: Schematic of how Mass Spectrometer works

Fig. 14.3/13.3 

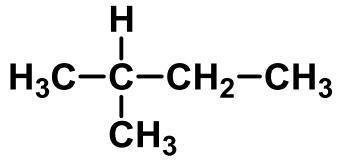
MW = 72 g/mole

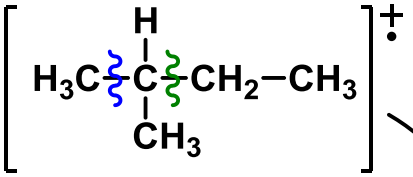


Highest mass peak = 72 ⇨ molecular ion = whole molecule but charged (M^+)

Other Peaks: lower mass = fragmentation peaks
M^+ extremely high energy, breaks into smaller bits

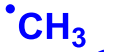
Tallest Peak = Base Peak
= most stable cation (can be M^+ or fragment)
= set to 100%, everything else is relative to it

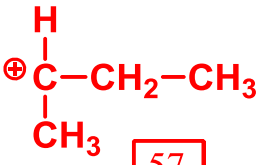
Fragmentation of 



$M^+ = 72$

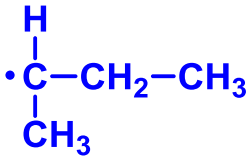
break


neutral,
don't see


57

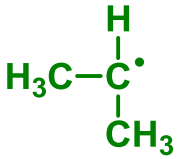
or

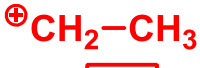

15



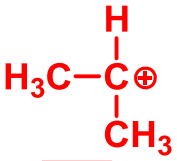
one bond has only one e^-
so breaks easily to give + and •

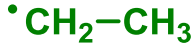
break




29

or


43



57 > 15 because 2° C^+
more stable

43 > 57 because both 2° C^+
but 43 has more stable radical

so 43 = base peak