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PLEASE COMPLETE NOTES IN INK AND DO NOT STAPLE.

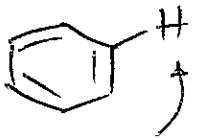
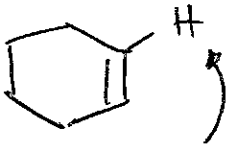
Recall: Benzene – an "aromatic" molecule

can think of it as  , but don't draw it this way.

•Spectroscopy

1) IR spectroscopy – see text

2) NMR spectroscopy: ^1H NMR: H's ~~on~~ on benzene have a characteristic downfield chemical shift (~7 ppm)

ex  vs 

δ 7.4 δ 5.7 ppm

~1.5-2 ppm downfield of alkenes

Explanation – large local magnetic field from induced circulation of aromatic π e⁻'s (Fig 16.2); analogous to alkenes

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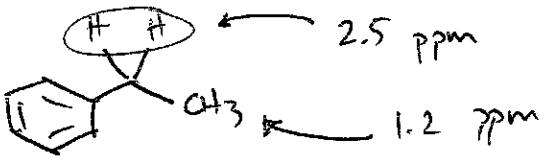
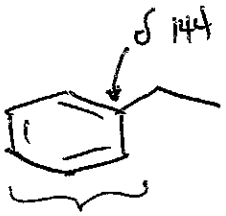
- Benzylic H's are also somewhat downfield



(Analogy to allylic H's)

- ^{13}C NMR: Aromatic C's show up in δ 110-160

Ex:



δ 125-128

- Chapter 16.3D - skip

- Reactivity! Electrophilic aromatic substitution

-In general, aromatic π systems are less reactive as nucleophiles than alkene π systems because the aromatic systems lose aromaticity (at least temporarily) during the course of the reaction.

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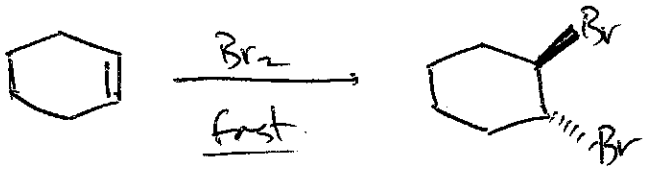
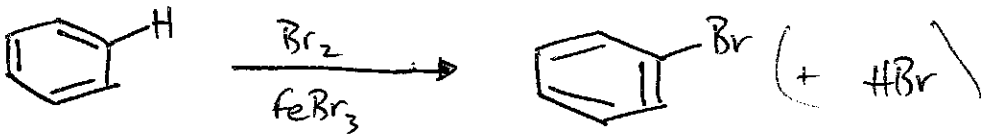
Example:



• If we make the electrophile more reactive, then a reaction will occur.

- Add Lewis acid catalyst to activate Br_2



* Key to this and all other EAS reactions is to generate a suitably reactive electrophile.

Thus,

more electrophilic than Br_2

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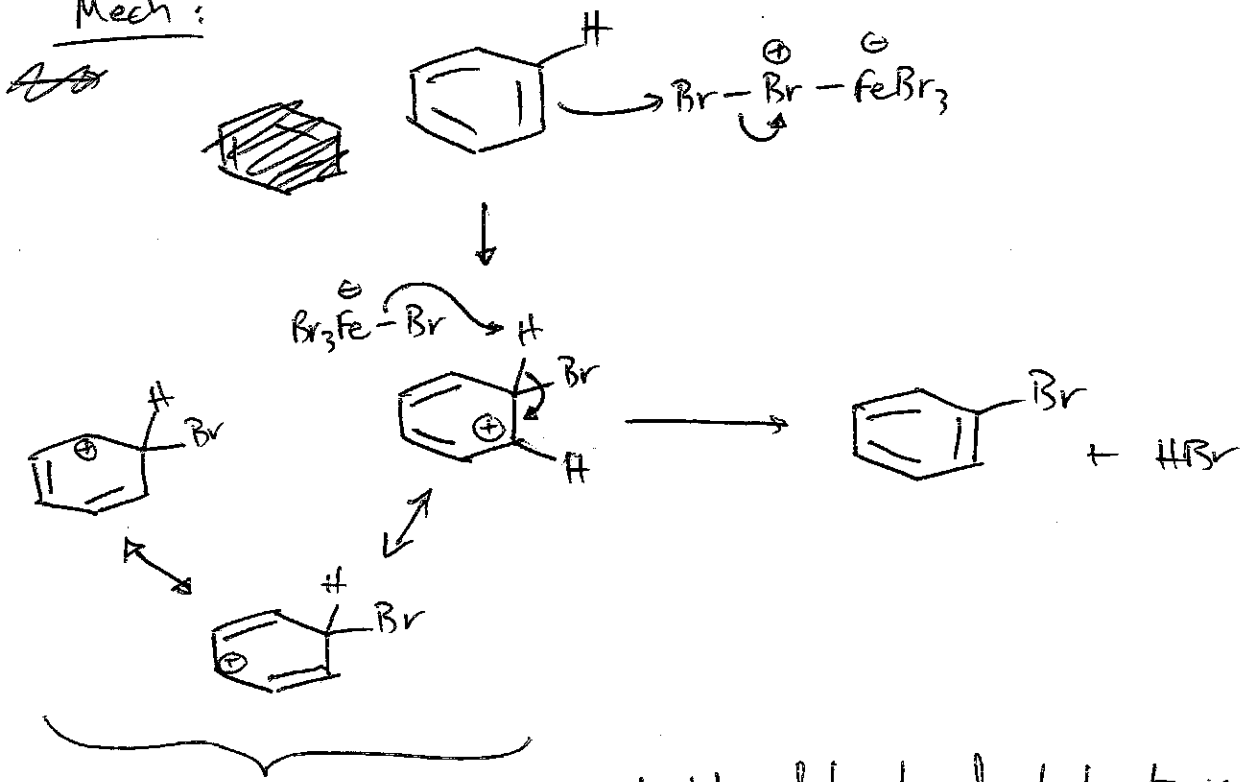
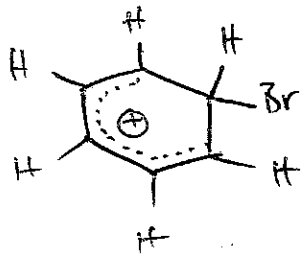
Mech:



the cationic intermediate is highly delocalized, but it is not aromatic

- Another image for this intermediate:



(don't use this when writing a mechanism)

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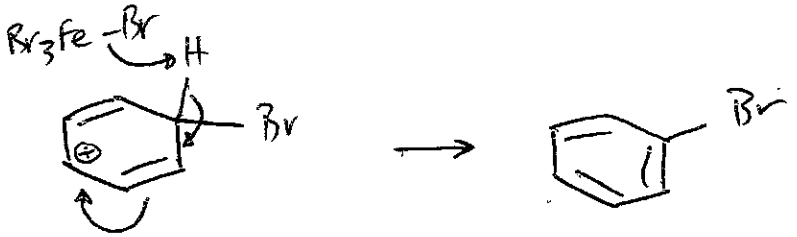
* Note: Do not use ~~⇌~~ curved arrows to "interconvert" resonance structures.

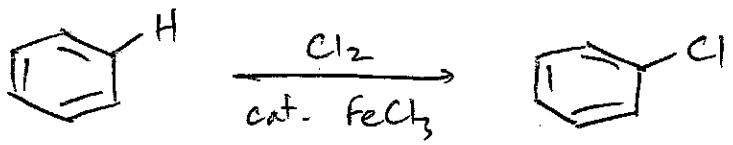
- If proper resonance structures are drawn, any can be used for the correct mechanism.

Ex:



* Many variations exist on EAS!

- Ex: chlorination



* Draw in the mechanism! *

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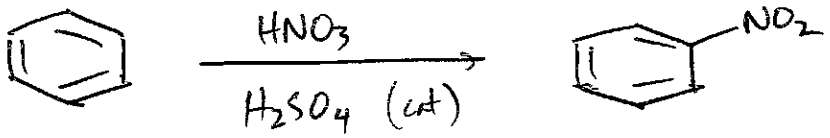
Nitration



• Nitro group: