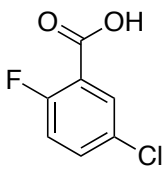
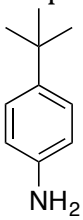
Chemistry 234
Chapter 15 Problem Set

Naming Aromatic Compounds

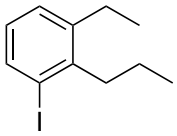
1) Provide the IUPAC name for each compound shown below.



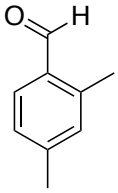
5-chloro-2-fluorobenzoic acid



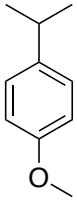
4-*tert*-butylaniline
or
p-*tert*-butylaniline



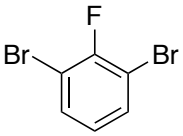
1-ethyl-3-iodo-2-propylbenzene



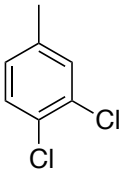
2,4-dimethylbenzaldehyde



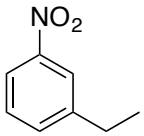
1-isopropyl-4-methoxybenzene
or
4-isopropylanisole
or
p-isopropylanisole



1,3-dibromo-2-fluorobenzene



1,2-dichloro-4-methylbenzene
or
3,4-dichlorotoluene



1-ethyl-3-nitrobenzene

Aromaticity

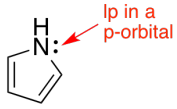
2) Classify each molecule below as aromatic, antiaromatic, or non-aromatic. For aromatic and antiaromatic compounds, give the number of π electrons in the ring.

Non-Aromatic

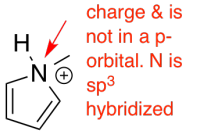
Aromatic
2π e-

There is debate over this one. If you consider the lp to be in sp^3 orbital this would be non-aromatic.

Antiaromatic
or Non-Aromatic
4π e-

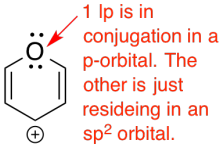


Aromatic
6π e-

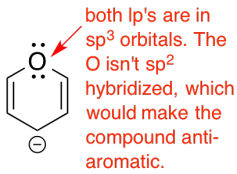


Non-Aromatic

Non-Aromatic

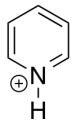


Aromatic
6π e-

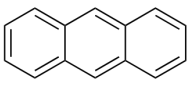


Non-Aromatic

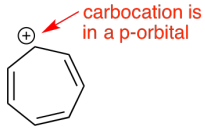
Aromatic
6π e-



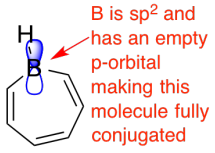
Aromatic
6π e-



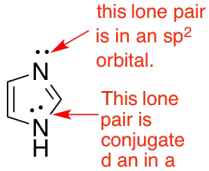
Aromatic
14π e-



Aromatic
6π e-



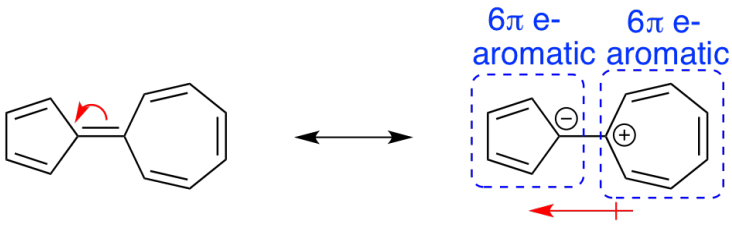
Aromatic
6π e-



Aromatic
6π e-

Non-Aromatic

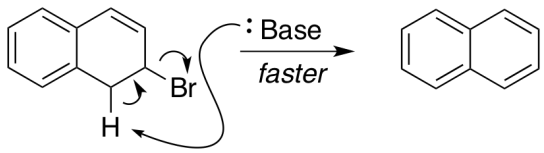
3) The molecule below has an unusually large dipole. Explain.



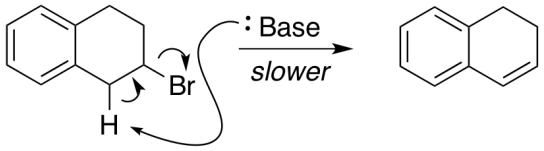
This is the major resonance contributor due to aromaticity. This resonance structure has a positive charge and negative charge adjacent to one another giving the molecule a large dipole moment.

4) Use your knowledge of resonance, aromaticity, and general stability trends to analyze the following reactions or trends.

a.

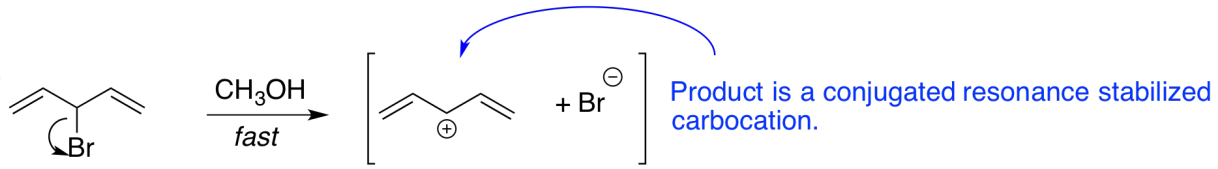


This elimination reaction occurs at a faster rate because you gain additional aromaticity stabilization in the product.

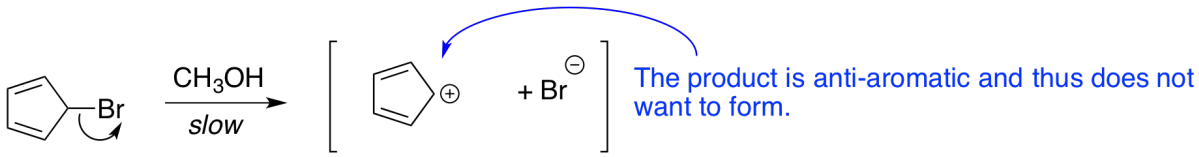


Although the alkene you get in the product is stabilizad by conjugation, you don't get a second aromatic ring in this reaciton.

b.

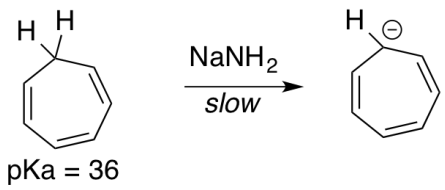


Product is a conjugated resonance stabilized carbocation.

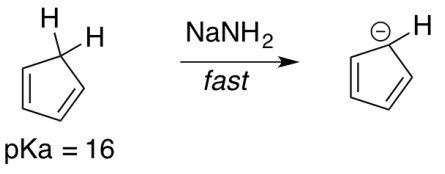


The product is anti-aromatic and thus does not want to form.

c.

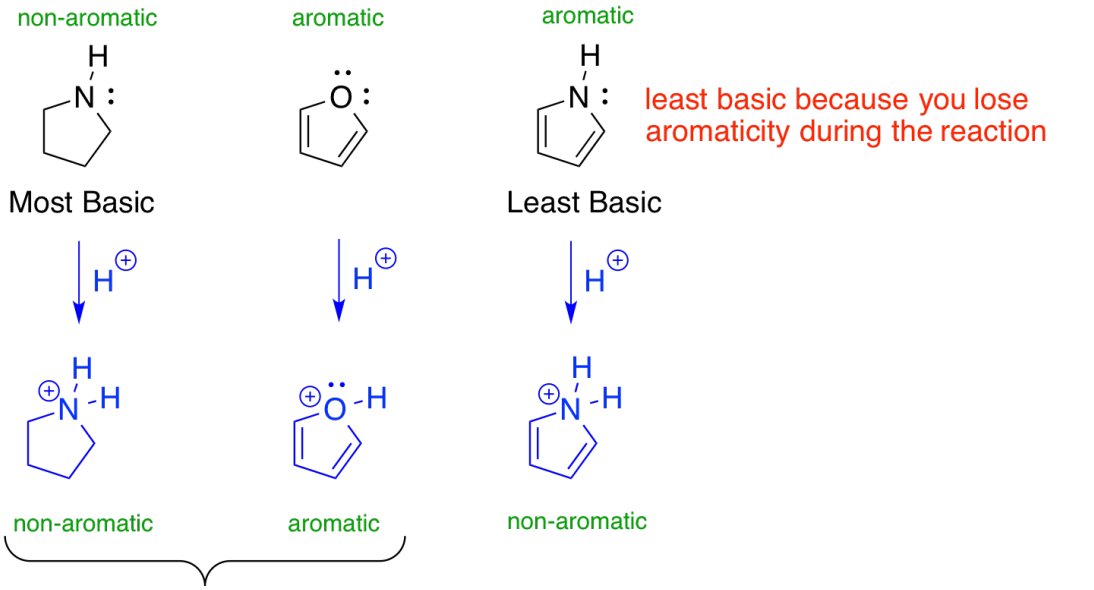


Non-aromatic



Aromatic (faster reaction because product is extra stable)

e.

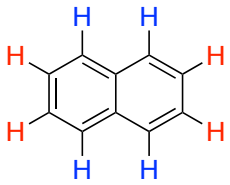


least basic because you lose aromaticity during the reaction

Both reaction have no net "aromaticity" change. The first goes from non-aromatic to non-aromatic and the second goes from aromatic to aromatic. The only compairson we can make is by the fact that O is more electronegative and holds its electrons more tightly making it less basic than the amine.

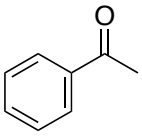
Spectroscopy

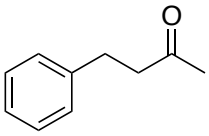
5) Construct a simulated ^{1}H NMR Spectrum of the aromatic compound naphthalene.

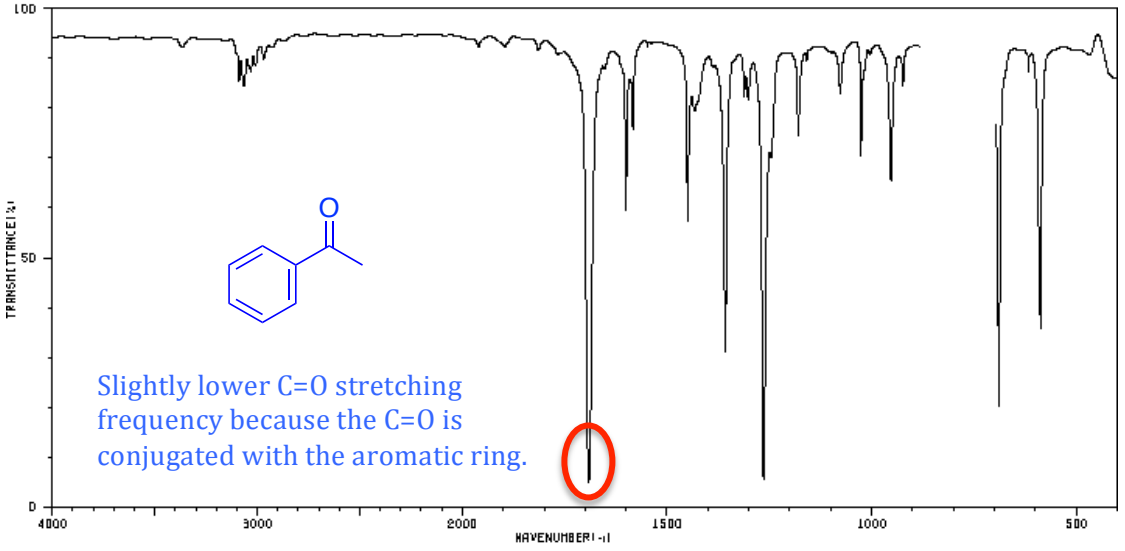


Would expect two doublets in the aromatic region (7-8 ppm) each integrating for 4H.

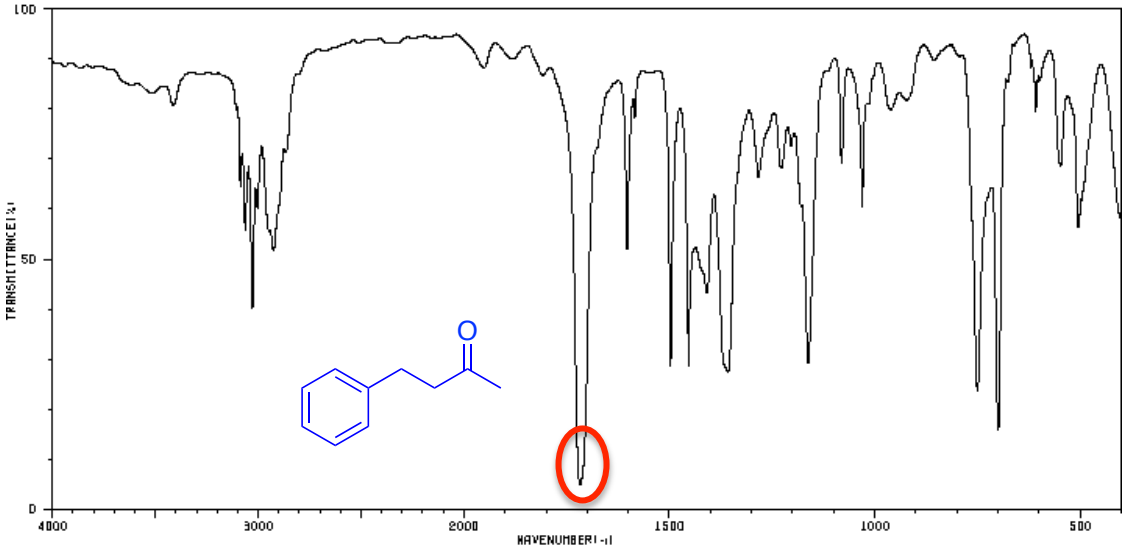
6) IR Spectra for two aromatic compounds are shown below. Match each compound to its corresponding IR spectrum and explain your reasoning.



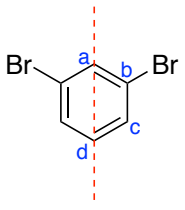




Slightly lower C=O stretching frequency because the C=O is conjugated with the aromatic ring.



7) Determine the number of distinct ^{13}C NMR signals for each compound below.



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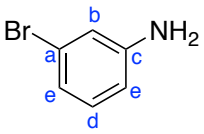
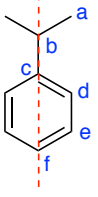
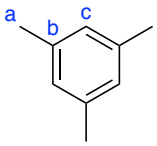


6



6



3

8) Draw a structure that corresponds to each 1H NMR spectrum shown below.