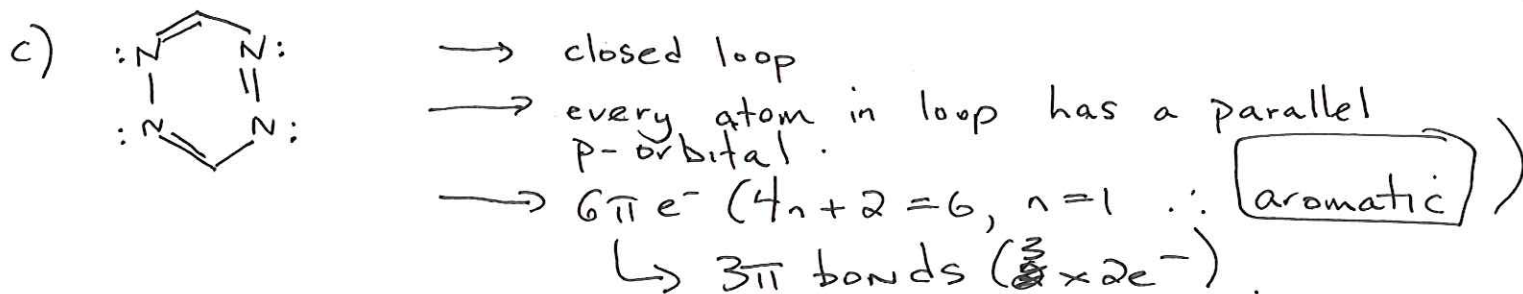
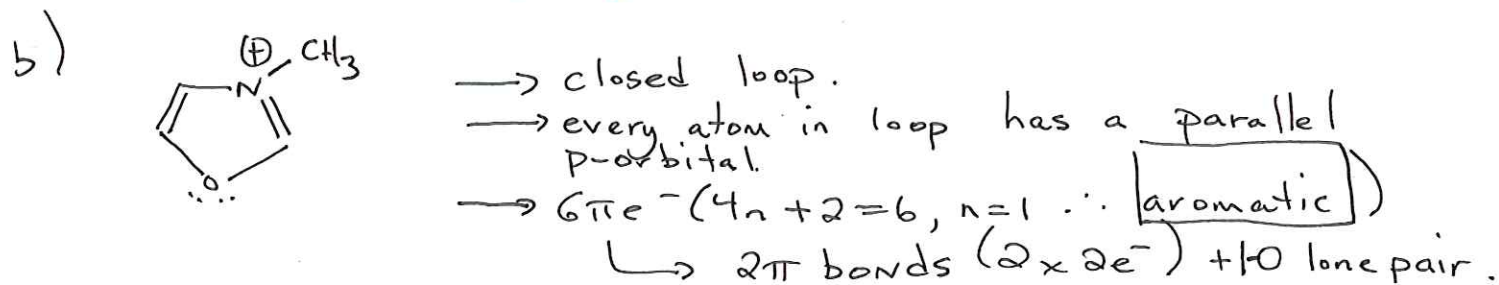
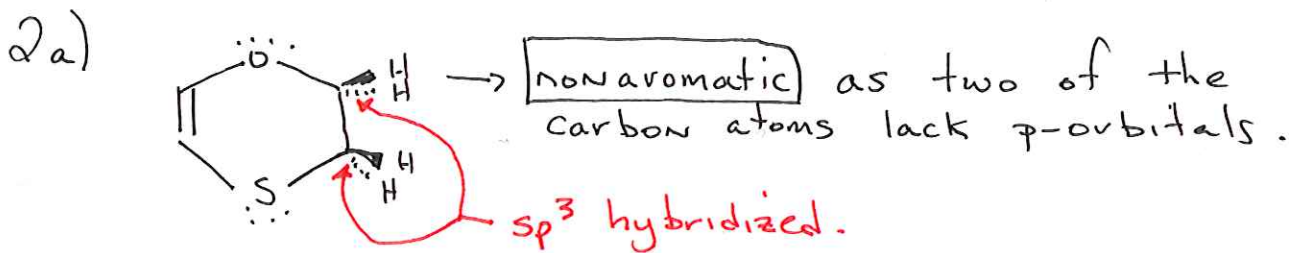
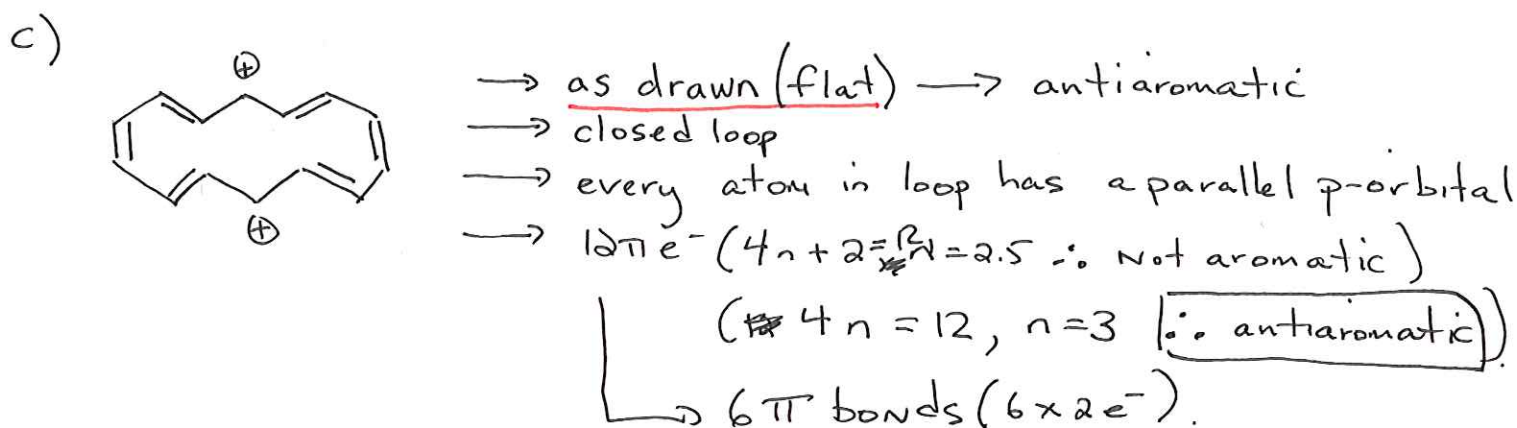
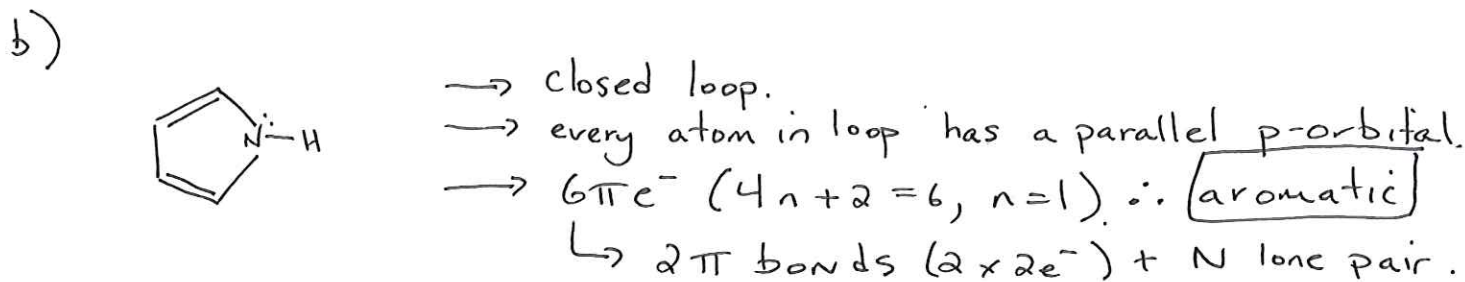
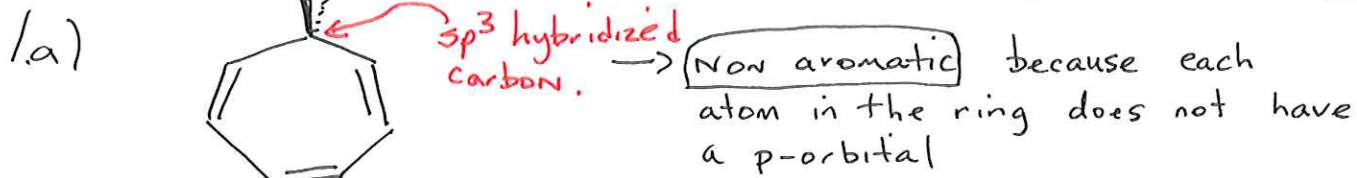
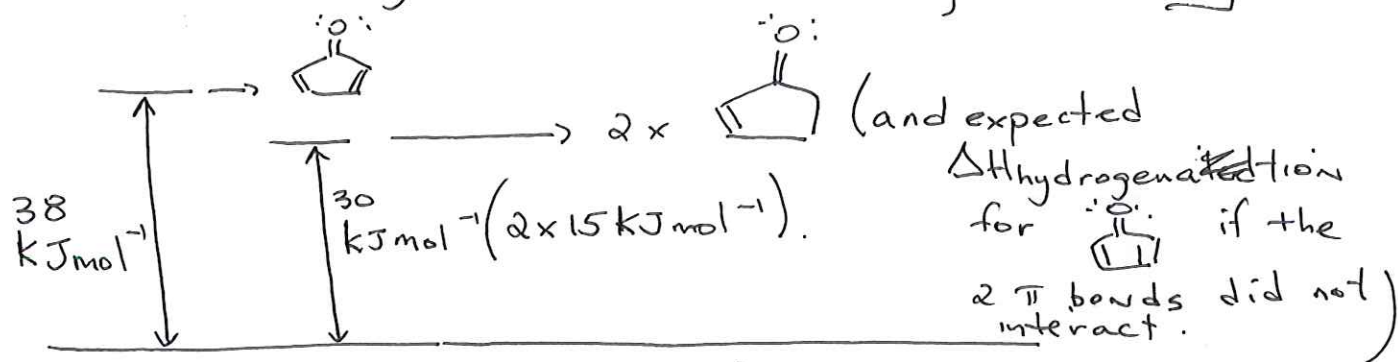


## Assignment #10 - Aromaticity - Answer Key



## Assignment #10 - Aromaticity Answer Key

3a).



→ Given that  $\Delta H_{\text{hydrogenation}}$  for cyclopentenone is  $15 \text{ kJ mol}^{-1}$ , one would expect hydrogenation of 2 double bonds to have twice this value (if there was interaction between the two double bonds).

$$\rightarrow 2 \times 15 \text{ kJ mol}^{-1} = 30 \text{ kJ mol}^{-1}$$

→ however, the  $\Delta H_{\text{hydrogenation}} \neq 30 \text{ kJ mol}^{-1}$  for cyclopentadienone.

→  $\therefore$  the 2  $\pi$  bonds must interact, and the difference between the actual and expected  $\Delta H_{\text{hydrogenation}}$  can be considered our "resonance energy".

$$\rightarrow -38 \text{ kJ mol}^{-1} - -30 \text{ kJ mol}^{-1}$$

$$= -8 \text{ kJ mol}^{-1}$$

$$(2 \times 15 \text{ kJ mol}^{-1}) \overset{\text{or}}{\rightarrow} -38 \text{ kJ mol}^{-1}$$

$$= -8 \text{ kJ mol}^{-1}$$

b) → The value calculated in part a) is negative, indicating that cyclopentadienone is higher in energy than one would expect (see figure in part a).

$\therefore$  cyclopentadienone can be considered to have antiaromatic character.

→ if the "resonance" energy were positive, it would indicate a ~~more~~ lower ground state energy than expected, and hence, aromatic character.

Chem 2500  
Assignment #10 - Aromaticity - Answer Key.

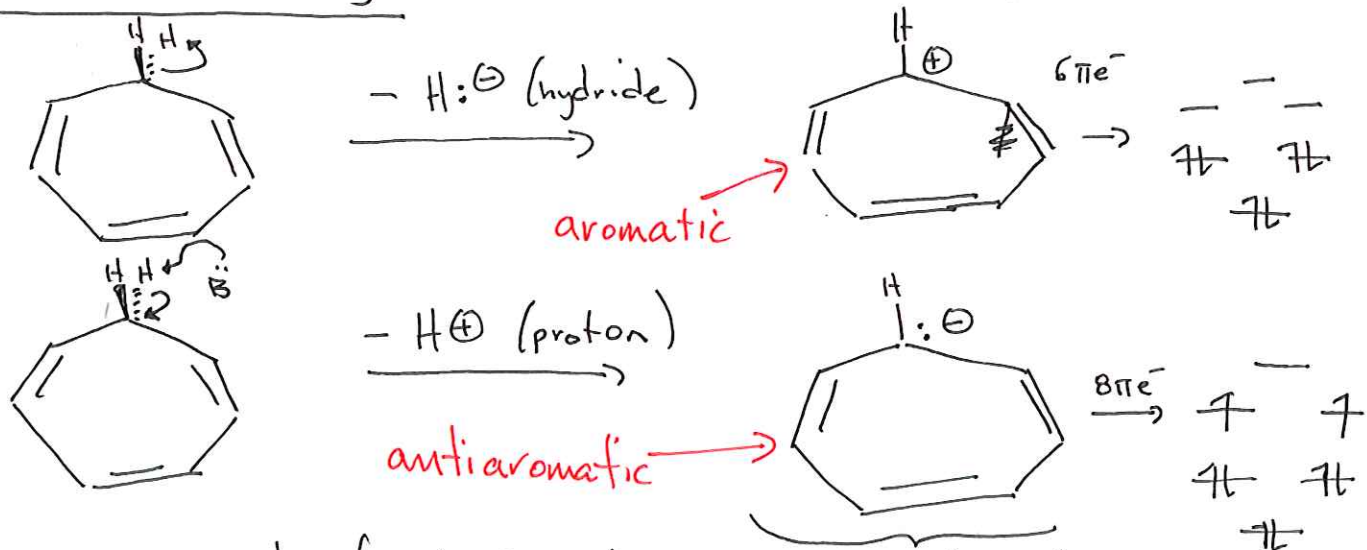
3c)



d) → the resonance structure in part c) meets the criteria of antiaromatic  
 → adjacent, co-planar p-orbitals at every atom in ring  
 →  $4n = 4, n=1$  ( $4\pi e^-$ ).

→ given that the weighted average of these two resonance structures places a partial  $\oplus$  charge on the carbonyl carbon, it is reasonable to describe cyclopentadienone as having antiaromatic character.

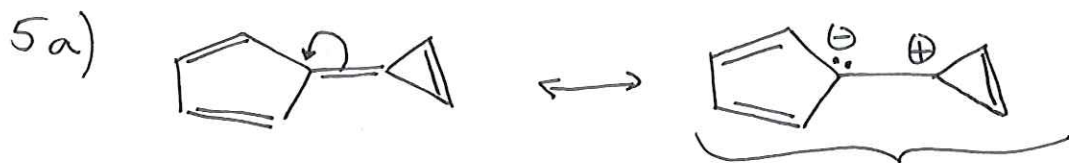
4.



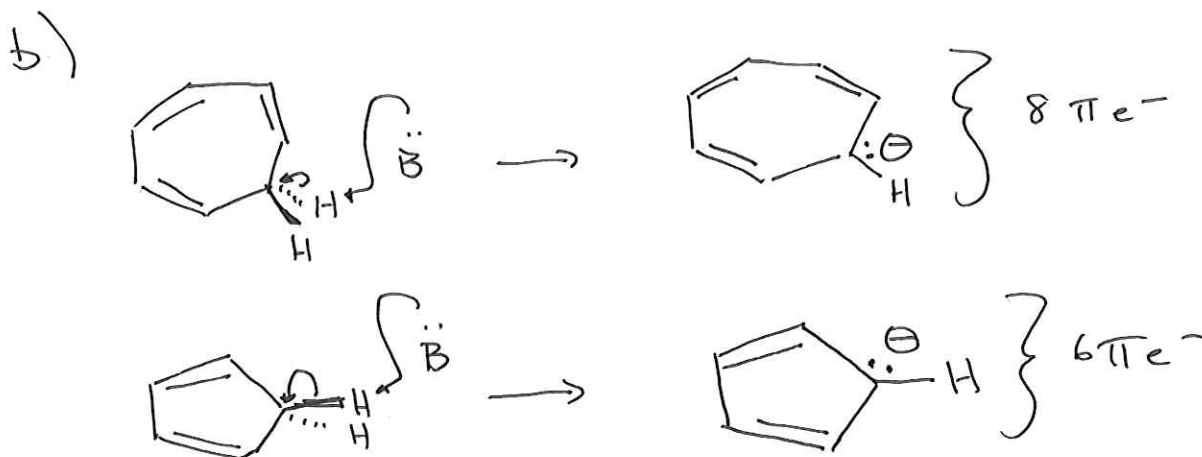
→ removal of  $H:\ominus$  gives an aromatic molecule (all bonding orbitals are filled) whereas removal of  $H\oplus$  gives antiaromatic diradical ( $2e^-$  in antibonding orbitals).  
 assuming anion is flat and lone pair is in a p-orbital.

↳ removal of a hydride is much more likely.

Chem 2500  
Assignment #10 Aromaticity - Answer Key.



This resonance structure is highly favoured as it makes both rings aromatic.



The top structure would be antiaromatic if planar and non-aromatic if puckered (or  $sp^3$  hybridized at  $C:\ominus$ ).

The bottom structure, however, is aromatic. Thus, cyclopentadiene is more acidic.