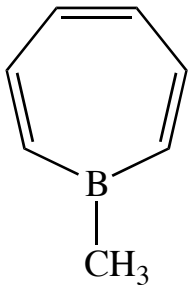
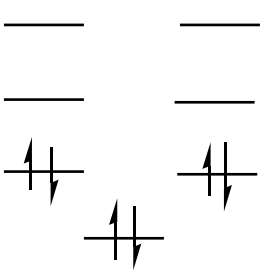
Exercise 112 - Arom/Anti/Non

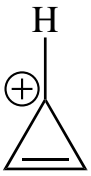
Question One



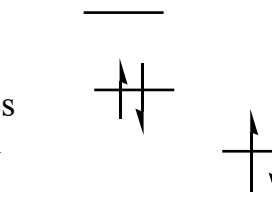
6 pi-electrons. The B atom is sp2 hybridized and has an empty atomic p orbital. This molecule is isoelectronic with the aromatic tropylium cation.

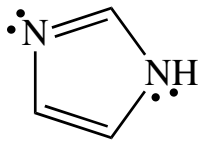
pi MO diagram



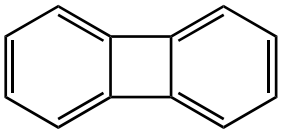


The cyclopropyl cation fits the Hückel rule for n = 0 i.e. 2p i-electrons.
It is aromatic.

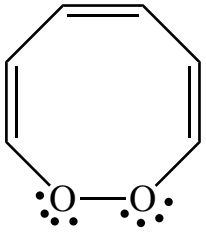




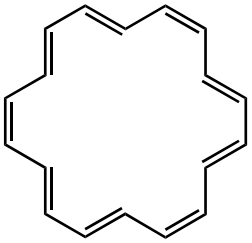
Imidazole, isoelectronic with pyrrole is aromatic. Note that the N bearing an H contributes it's lone pair to the aromatic pi cloud but the other N does not since it is already involved in a pi bond with an adjacent carbon. 6 pi electrons.



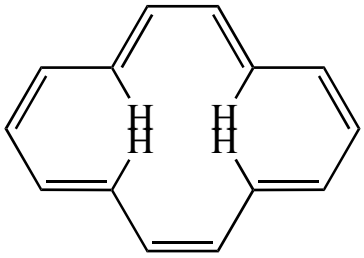
Biphenylene is a 12 pi-electron system that is anti-aromatic. It is a fairly stable species though. The two benzene substructures actually try to isolate themselves so this molecule has some of the character of an aromatic biphenyl.



I'm not sure if this molecule is known. As a peroxide, it is likely rather reactive. Each O atom contributes 2 pi-electrons for a total of 10, so one might expect this molecule to be aromatic. It is isoelectronic with the cyclooctatetraene dianion which is certainly aromatic.



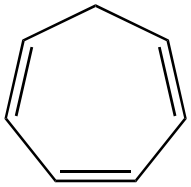
18-Annulene is a fascinating molecule that fits all the criteria for aromaticity. The H atoms in the interior can fit without too much steric interference. This molecule has an amazing NMR spectrum.



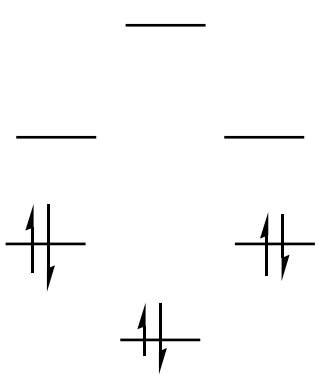
Though the electron count fits the Rule, the steric interactions of the interior H atoms prevents this molecule from being sufficiently planar to be aromatic.

Question Two

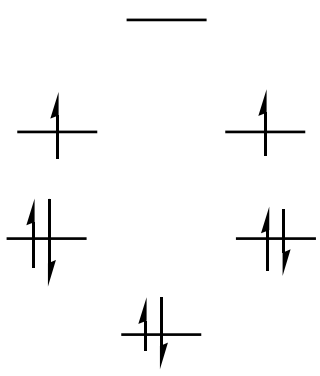
Removal of hydride (H-) or a proton from cyclononatriene below gives an anion or cation. Which process is more likely? Sketch the pi MO diagrams for both species as part of your answer.



The cation (removal of H-) is the aromatic tropylium ion, so this is the favoured process.



Cation - 6 pi electrons



Anion - 8 pi electrons

Note that the anion is a diradical while the cation has filled bonding orbitals.