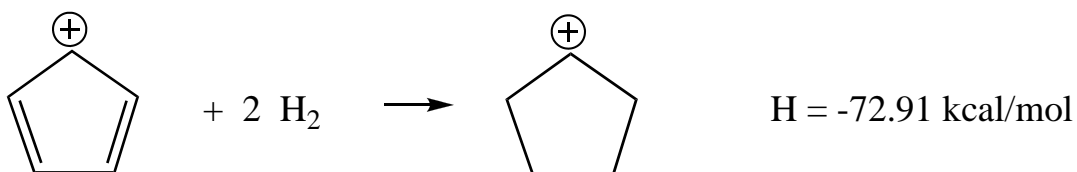
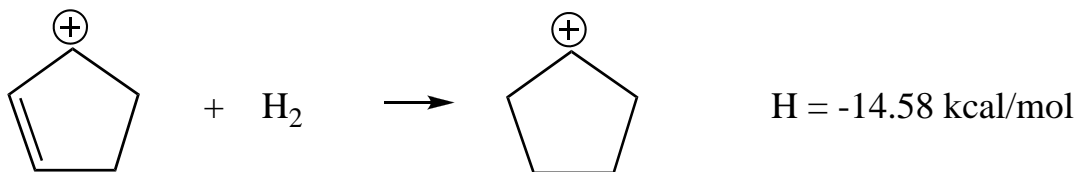


Exercise 111 - Res Energy/MO

Question

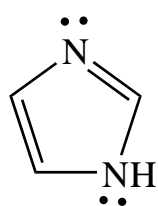
From the following, calculate the resonance energy of the cyclopentadienyl cation.



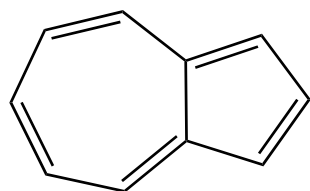
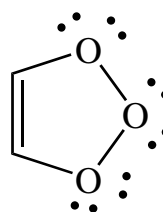
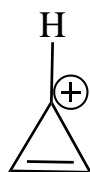
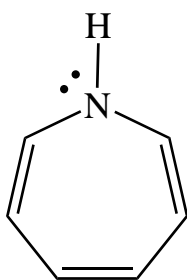
Sketch the MO diagram for this species and use it to determine whether this is an aromatic or antiaromatic molecule. Is this consistent with the resonance energy?

Question

Sketch MO diagrams for the following molecules/ions and use them to predict whether they are aromatic or antiaromatic.



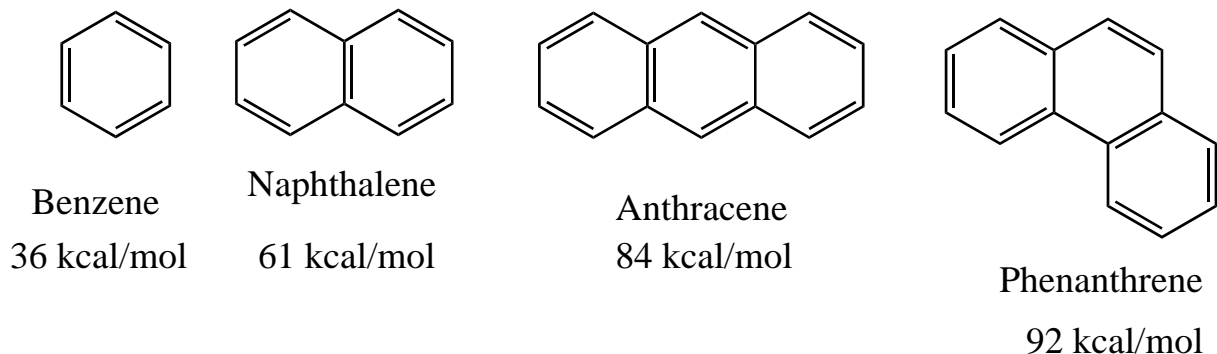
Imidazole



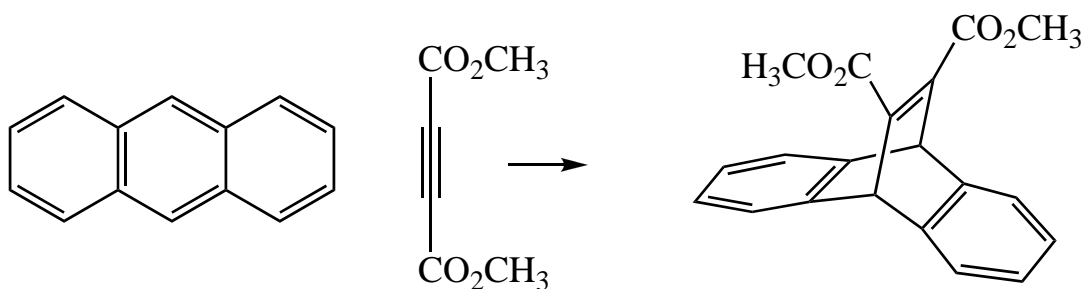
Azulene

Question Four

i) Shown below are the structures of the first four benzene-based aromatic hydrocarbons and their associated resonance energies. Calculate the REPE (resonance energy per pi electron) for each one. What do you notice?



ii) Benzene and naphthalene do not undergo addition reactions. Anthracene, however, will react as a Diels-Alder diene:



Why does this reaction occur but not the corresponding reaction with benzene or naphthalene? Hint: compare the resonance energies of the product and reactant.

iii) Phenanthrene has five Kekulé resonance structures. One of the bonds of phenanthrene reacts with bromine to give an *addition reaction* just like an alkene. Which bond? Explain.

