Objectives

After completing this section, you should be able to draw the resonance contributors for polycyclic aromatic compounds, such as naphthalene, anthracene, etc.

Key Terms

Make certain that you can define, and use in context, the key term below.

- polycyclic aromatic compounds

Study Notes

As their name indicates, *polycyclic aromatic hydrocarbons* are aromatic hydrocarbons which contain more than one benzenoid (i.e., benzene-like) ring. This section deals only with those compounds in which the benzenoid rings are fused together; in other words, compounds in which at least one carbon-carbon bond is common to two aromatic rings. Another type of polycyclic aromatic hydrocarbon contains two or more benzenoid rings joined by a carbon-carbon single bond. The simplest compound of this type is biphenyl, the compound from which PCBs (polychlorinated biphenyls) are derived.

- biphenyl and 2,4,2',5'-tetrachlorobiphenyl

**Figure 15.3**: Structures of biphenyl and a typical PCB

**Aromatic Compound with a single ring**

<table>
<thead>
<tr>
<th>Unstable Planar Configurations</th>
</tr>
</thead>
<tbody>
<tr>
<td>• transannular crowding in trans-isomer</td>
</tr>
<tr>
<td>• angle strain (240° total) in cis-isomer</td>
</tr>
</tbody>
</table>

**Aromatic Compounds with more than one ring**

Benzene rings may be joined together (fused) to give larger polycyclic aromatic compounds. A few examples are drawn below, together with the approved numbering scheme for substituted derivatives. The peripheral carbon atoms (numbered in all but the last three examples) are all bonded to hydrogen atoms. Unlike benzene, all the C-C bond lengths in these
fused ring aromatics are not the same, and there is some localization of the pi-electrons.

The six benzene rings in coronene are fused in a planar ring; whereas the six rings in hexahelicene are not joined in a larger ring, but assume a helical turn, due to the crowding together of the terminal ring atoms. This helical configuration renders the hexahelicene molecule chiral, and it has been resolved into stable enantiomers.

![Figure 2: Examples of Polycyclic Aromatic Hydrocarbons (PAHs).](image)

Exercises

Questions

Q15.6.1

This is an isomer of naphthalene. Is it aromatic? Draw a resonance structure for it.

![Structure](image)

Q15.6.2

The following molecule is adenine. It has a purine core. Of the nitrogen in the core, how many electrons are donated into the pi system?
Solutions

S15.6.1

Yes, it is aromatic. 4n+2 pi-electrons.

\[ \begin{align*}
\text{Octahedral} & \quad \leftrightarrow \quad \text{Planar}
\end{align*} \]

S15.6.2

There is only one nitrogen of the core that contributes to the pi-system (in red). With this one lone pair the core is aromatic with 10 electrons in the pi-system.

Contributors

- Dr. Dietmar Kennepohl FCIC (Professor of Chemistry, Athabasca University)
- Prof. Steven Farmer (Sonoma State University)