Resonance Structures
The Benzene $\pi$ System

- Each carbon in benzene is trigonal planar and $sp^2$ hybridized.
- Hence, all of the $p$ orbitals in benzene are parallel and readily overlap.
Aromatic Compounds

Benzene
Pyridine
Pyrole
Furan

Napthalene
Quinoline
Azulene
Purine
Pyrimidine

DNA Bases

Adenine
Guanine
Cytosine
Thymine
Uracil (RNA)

Amino Acids

Phenylalanine
Histidine (Imidazole)
Tryptophan (Indole)
Tyrosine (Phenol)
Graphite

- Graphite is a form of elemental carbon that consists of layers of fused benzene rings.
- It is an excellent electrical conductor because of the ease at which the $\pi$-electrons can delocalize.

Buckminsterfullerene

- All 60 of the carbons are equivalent.
- Nicknamed “buckyballs.”
Physical Basis of UV-Vis Spectroscopy

- UV-vis is based on excitation of \( \pi \) electrons.
- The energy required for absorption must match the \( \Delta E \) between \( \pi \) and \( \pi^* \).
UV-Vis Spectroscopy of Conjugated Systems

- The HOMO-LUMO gap becomes smaller as the number of conjugated double bonds increases.
IR Spectroscopy

(a) Benzene derivatives
- C=C stretch
- C–H bending
- Overtones and combination bands

(b) Phenol derivatives
- O–H stretch
- C–O stretch

Percent transmittance
Wavenumber, cm⁻¹
Wavelength, micrometers
Substituted Benzenes

Adrenaline (epinephrine)
- Active agent of the peyote cactus
- Bronchodilator

Mescaline

Ephedrine
- Agent Orange
- Substituted benzenes

Fenfluramine

Phentermine

Saccharin

Amphetamine

Methamphetamine

Discovered/synthesized by chemists

MDMA "Ecstasy"

Serotonin
signature for para-substitution

distinct from ortho-substitution
Average: 111.58/150 = 74.4% with a standard deviation of 16.4.