

Molecular Modeling Shapes & Orbital Hybridization

Quantum Mechanics: Molecular Orbital Theory

Quantum mechanics describes the energy in terms of interactions among nuclei and electrons. This is given by the Schrödinger equation.
The Schrödinger equation may be solved exactly for the hydrogen atom.

$$H\psi = E\psi$$

H = Hamiltonian

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(x,y,z)\psi = E\psi(x,y,z)$$

kinetic energy potential energy total energy

$\psi(x,y,z)$ = wavefunction describing the system.

Its solutions are very familiar to chemists as atomic orbitals.

H is an operator corresponding to the total energy of the system.
Kinetic + potential energy

Web MO

<http://butane.cabrillo.edu/>
Username: your last name
password: DVC id#

Output:

- ❖ Dipole moment
- ❖ Bond Orders
- ❖ Electron Density
- ❖ Partial Charges
- ❖ Vibrational Modes
- ❖ Molecular Orbitals
- ❖ Ultraviolet-Visible-Infrared Graphics
- ❖ NMR Chemical Shifts

Hydrogen Halides

Hydrogen-Halogen Bond Lengths and Bond Strengths			
Hydrogen halide	Bond length (Å)	bonded	liberal
H-F	0.917	136	571
H-Cl	1.2740	103	432
H-Br	1.4143	87	366
H-I	1.6090	71	298

Molecular Dipole Moment

The vector sum of the magnitude and the direction of the individual bond dipoles determines the overall dipole moment of a molecule

carbon dioxide $\mu = 0$ D

carbon tetrachloride $\mu = 0$ D

chloromethane $\mu = 1.87$ D

water $\mu = 1.85$ D

ammonia $\mu = 1.47$ D

CH_2Cl_2 molecule CCl_4 molecule

An electrically charged rod attracts a stream of chloroform but has no effect on a stream of carbon tetrachloride.

Molecular Polarity

- Consider the resultant dipole for CH_3Cl
- Dipole moment (μ) = charge (e) x distance (d)

Polarity & Physical Properties Ozone and Water

0.1278 mD

Resultant Molecular Dipoles > 0

- Solubility: Polar molecules that dissolve or are dissolved in like molecules
- The Lotus flower
- Water & dirt repellancy

The "Lotus Effect" Biomimicry

<http://bfh.org/biomimicry>

- Lotus petals have non-polar wax on its micrometer-scale rough surface, resulting in water contact angles up to 150°
- See the middle image above.
- When it rains, water dissolves any polar materials on the surface and gravity takes care of any insoluble, non-polar "dirt" on the lotus surface, much like a snowball.

Hybridization

Mixing Atomic Orbitals

Hybridization of s and p orbitals

Hybridization

<http://www.chem.uiuc.edu/CLTutorials/104/Hybridization/SeeIt.html>

Single Bonds (Methane)

Hybridization of s and p atomic orbitals:

The atomic orbitals used in bond formation determine the bond angles

• Tetrahedral bond angle = 109.5°

• Electron pairs spread themselves into space as far from each other as possible. The single bond is called a sigma bond (σ) with a bond order of 1.

Double Bond: sp^2 -Hybridized Carbon

• A double bond consists of one sigma (σ) bond and one pi (π) bond with a bond order of 2.

• Double bonds are shorter and stronger than single bonds

• The bond angle of the sp^2 carbon is ~ 120° (Trigonal Planar)

Ethyne: A Triple Bond sp -Hybridized Carbon

• A triple bond consists of one σ bond and two π bonds with a bond order of 3.

• Triple bonds are shorter and stronger than double bonds

• There is a bond angle of the sp carbon: 180° (linear)

Hybridization & Bond Strength

	ETHANE	ETHYLENE	ACETYLENE
Structure			
C-C bond length	1.54 Å	1.34 Å	1.20 Å
Bond energy	348 kJ/mol	632 kJ/mol	820 kJ/mol
Bond Order	1	2	3

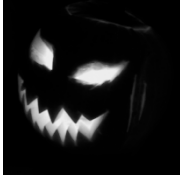
Light & The Chemistry of Vision

Color Blind & Vampires

B&W vs. Color vision : Rods vs. Cones

PALM OF YOUR EYE Vision is triggered when light isomerizes rhodopsin's 11-cis-retinal-derived cofactor to the trans form. A series of enzyme-catalyzed steps are then required to regenerate the 11-cis-retinal cofactor. Palmitoylated RPE65 plays two crucial roles in this cycle. LRAT uses it as a palmitoyl donor to make all-cis-retinyl palmitate from vitamin A, and palmitoylated RPE65 (but not the unmodified protein) delivers all-cis-retinyl palmitate to the next enzyme in the cycle.

Halloween / All Hallows Eve



*Have you donated blood?
Planning a vampire encounter?
Is Bram Stoker's "Dracula" pure
fiction?*

What follows *All Hallows Eve*?



Day of the Dead

The Link Between the Two Days?



Vampires & Porphyria?
Edward Munch.

Porphyria

Erythropoietic porphyria symptoms: severe photosensitivity, swelling, pain, and burning; requires avoidance of bright sunlight; produces brown canine teeth that fluoresce in ultraviolet light; produces hemolytic anemia. Drinking large quantities of blood can alleviate the symptoms. Garlic activates an enzyme that destroys them faster and makes the symptoms of porphyria worse.

<http://en.wikipedia.org/wiki/Porphyria>

Q. "Why is a baby like a vampire?"

A "Because it sleeps all day and feeds all night."