

Introduction and Review

1) **A Brief Introduction** (source: Lecture Supplement: Introduction and Review, pg 1)

a) Organic Chemistry-focuses on carbon containing molecules

b) Special Properties of Carbon:

- Able to form stable chains and rings
- Basis of life (important to biology)

2) **Molecular Structure** (source: Lecture Supplement: Introduction and Review, pg 2)

Molecular structure has two components:

- Electron distribution (bonds)
- Positions of atoms in space

Representing Molecular Structure: Drawing Diagrams

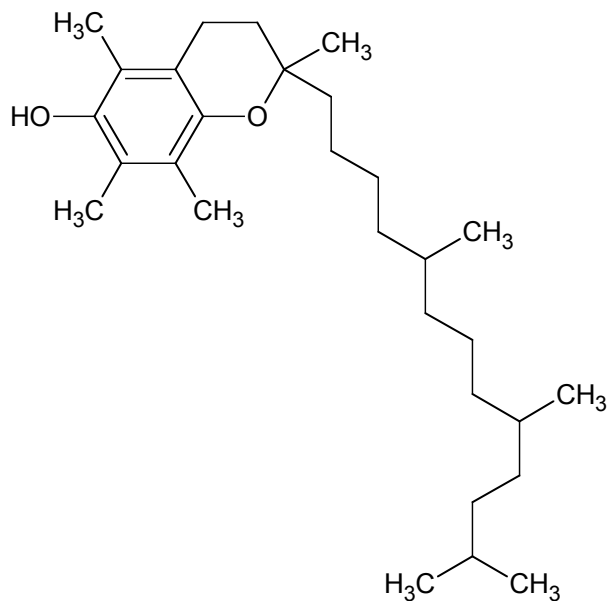
- Carbons are not drawn-in
- Hydrogens are omitted if carbons are not shown
- Any other atom is shown by its symbol
- Lone pairs are not always shown
- Formal Charges are always written-in
- Solid wedges indicate that the bond is pointing out of the page
- Hatched wedges indicated that the bond is pointing into the page

Example 1)

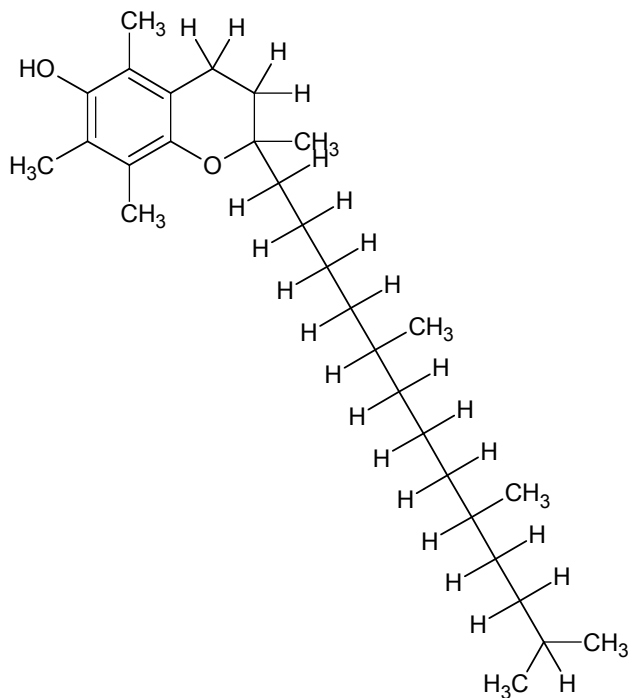
a) Label all of the missing hydrogens in Vitamin E

b) Count the lone pairs

c) Give the formula



Vitamin E without hydrogens



a) Vitamin E with hydrogens

b) 4 lone pairs- two pairs on each oxygen

c) Formula: $C_{29}H_{50}O_2$

3) Counting Valence Shell Electrons

- H: full shell has 2 electrons
- 2nd row elements (CNOF): full shell has 8 electrons
 - Octet rule: atoms can have 8 valence shell electrons, resulting in a maximum of four bonds
 - Watch out for PENTAVALENT carbons!
- 3rd row elements: easily violate the octet rule (i.e. P=10, S=12)

4) Assigning Formal Charge (source: Bruice; Section 1.4; pg 13)

Formal Charge- the *difference* between the number of valence electrons of a free atom and the number of electrons belonging to that atom when it is bonded

$$F.C = V - (L + 1/2 B)$$

V=valence electrons
L=lone electrons
B=Bonding electrons

Example 2) Calculate the Formal Charge on oxygen that is part of the ether group in Vitamin E (see Example 1)

$$F.C = V - (L + \frac{1}{2} B)$$

$$V = 6$$

$$L = 4$$

$$B = 4$$

$$F.C = 6 - (4 + \frac{1}{2} * 4)$$

$$F.C = 0$$

5) Electron Distribution (sources: Bruice; Section 1.3; pg 10 and Lecture Supplement: Introduction and Review; Hardinger; pg 4)

- Even sharing of electrons-covalent bond
- Uneven sharing-polar covalent bond

Electronegativity- an atom's ability to attract electrons from other atoms in the same molecule

Using the Pauling Scale we have... FOCINBrISCPH

$$F = 4.0$$

$$O = 3.5$$

$$Cl = 3.0$$

$$Br = 2.8$$

$$I = 2.5$$

$$P = 2.1$$

$$N = 3.0$$

$$S = 2.5$$

$$H = 2.1$$

$$C = 2.5$$

- Fluorine is the most electronegative atom on the periodic table.
- Electronegativity *decreases* from right to left and from top to bottom on the periodic table.

6) **Bond Polarity** (Lecture Supplement: Introduction and Review; Hardinger; pg 4-5)

- Bond Polarity: An uneven sharing of electrons, yielding partial charges (δ^- or δ^+)
- More polar bonds (larger electronegativity difference between atoms) results in a dipole of higher magnitude
- The bond length between the atoms amplifies the affect of electronegativity, thus increasing the magnitude of the dipole.
- Bond polarity influences the physical/chemical/biological properties of a molecule.

7) **Molecular Geometry, Orbitals, Hybridization, Bond Rotation, Newman Projections**
(Lecture Supplement: Introduction and Review; Hardinger; pg 5-7)

a) **Hybridization (by Pauling)- involves COMBINATIONS of atomic orbitals**

- “*Stability causes geometry; geometry causes hybridization*” (Lecture Supplement; pg 6)
- Hybridization is a **RESULT** of geometry, NOT a CAUSE of geometry.
- The repulsion of electrons affects bond angle
- Lone pairs (:) count in hybridization schemes

Shape	Hybridization	Number of electron groups	Bond Angle
Linear	$sp + sp + p_x + p_z$	2	$\sim 180^\circ$
Trigonal Planear	$sp^2 + sp^2 + sp^2 + p_z$	3	$\sim 120^\circ$
Tetrahedral	$sp^3 + sp^3 + sp^3 + sp^3$	4	$\sim 109.5^\circ$

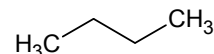
b) **Strain-** a decrease in the stability of a molecule caused by...

- **Angle Strain-** a deviation from ideal bond angles which results in strain on the molecule
- **Torsional Strain-** strain resulting from electron repulsion when groups of atoms get too close to one another
 - Cyclic molecules reduce torsional stain by adopting nonplanar conformations. For example, the chair conformation of cyclohexane.

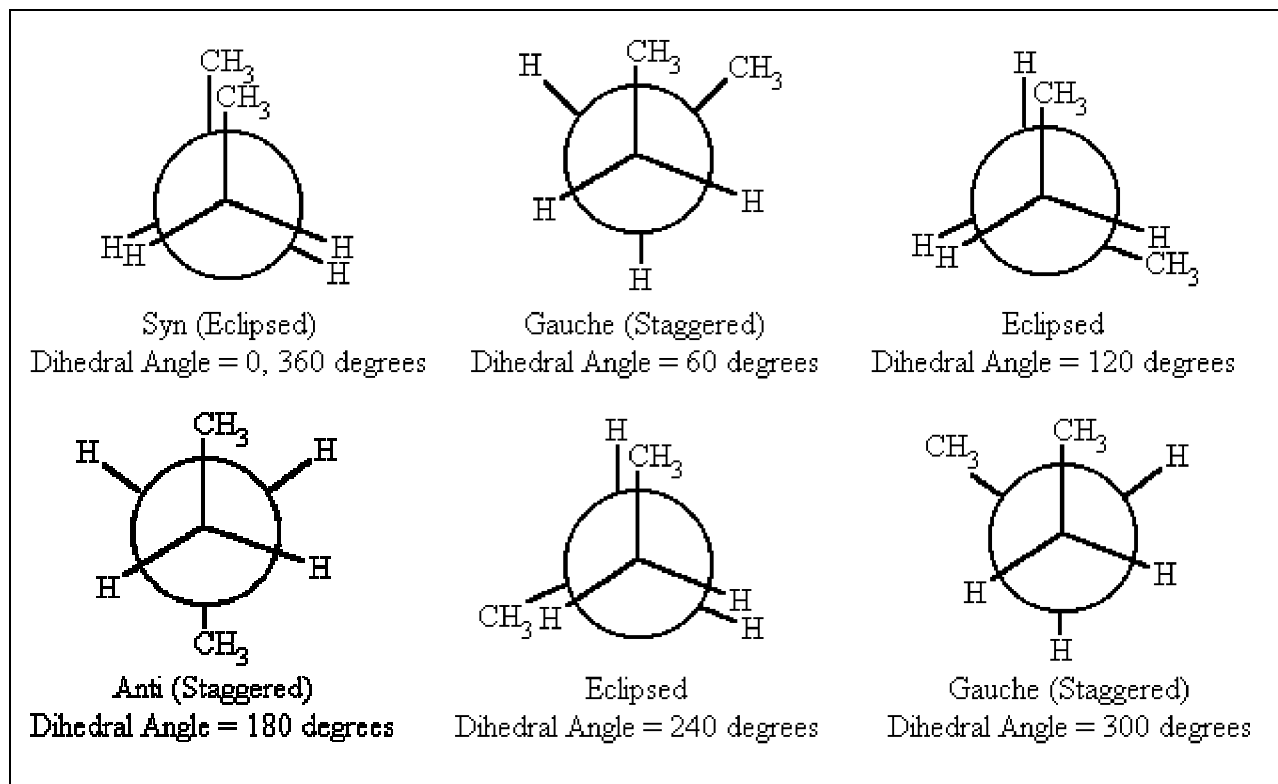
c) **Chair Conformation- Cyclohexane**

- Ring flip- axial \leftrightarrow equatorial
- Equatorial groups are preferred over axial groups because they have less torsional strain and therefore provide an increase in stability.

Skeletal Structure of
Butane:



d) Newman Projections for Benzene (C2-C3)



(Diagram source: http://www.cem.msu.edu/~cem251/F96/alkane_conformations/cem3.html)

Molecular models are very useful in visualizing Newman Projections as well as the chair conformation of cyclohexane.

Which conformation of butane is the most stable? Which is the least stable?

- The *anti* conformation is the *most stable* because it has the lowest amount of electron repulsion and the lowest amount of torsional strain. This is because the two largest groups (CH_3 's) are the farthest away from each other.
- On the other hand, the *eclipsed* conformation of butane is the *least stable* because it has the most electron repulsion and the most torsional strain since the CH_3 's are bumping into one another.