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5.111 Principles of Chemical Science  
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## Determining Hybridization in Complex Molecules:

See lecture 15 notes for a detailed discussion of hybrid orbitals. See page 1 of lecture 16 notes for a general rule to predict the hybridization of atoms with *s* and *p* electrons.

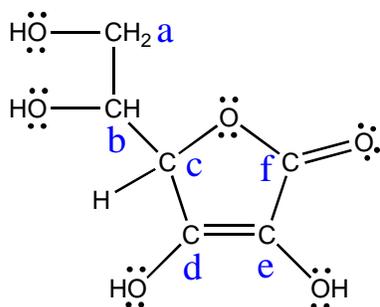
To determine the hybridization of a given atom in a molecule,

$$(\# \text{ of bonded atoms}) + (\# \text{ of lone pairs}) = \# \text{ of hybrid orbitals}$$

2 hybrid orbitals-  $sp$ ,      3 hybrid orbitals -  $sp^2$ ,      4 hybrid orbitals-  $sp^3$

Exception: single-bonded, terminal atoms. For the purposes of this course, do NOT hybridize single, bonded, terminal atoms.

### Example 1) from page 1 of Lecture 16 notes: Identifying the hybridization and geometry of atoms in ascorbic acid (vitamin C)



Identify the hybridization and geometry of each C atom:

$C_a$ :	$C_d$ :
$C_b$ :	$C_e$ :
$C_c$ :	$C_f$ :

Identify the symmetry ( $\sigma$  or  $\pi$ ) and name the hybrid or atomic orbitals that constitute the following bonds:

Bonds to carbon b:

$C_b$ -H:

$C_b$ -  $C_a$ :  $\sigma(C2sp^3, C2sp^3)$

$C_b$ - $C_c$ :  $\sigma(C2sp^3, C2sp^3)$

$C_b$ -O:

Bonds to carbon d:

$C_d$ -O:

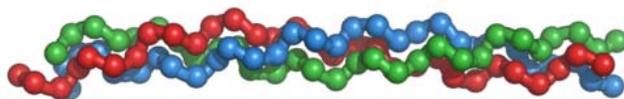
$C_d$ -  $C_e$ :  $\sigma(C2sp^2, C2sp^3)$

$C_d$ - $C_e$ :

Some interesting facts about vitamin C:

- Vitamin C is active in the body as the ascorbate ion. Like vitamin E, vitamin C is an antioxidant.
- Vitamin C is also an enzyme cofactor, meaning it that vitamin C binding is required for certain enzymes to function. Specifically, vitamin C is a required co-factor for enzymes that add hydroxyl groups to collagen, allowing the formation of the collagen triple

helix (pictured below). Since collagen is the main component of connective tissue, bones, cartilage, tendons, teeth, etc, it is clear that vitamin C is a very important molecule.



- Vitamin C deficiency is the cause of scurvy. Most people associate scurvy with boat travel in the 1500s to 1700s. Symptoms include irritated gums, tooth loss, bleeding from mucous membranes and eventual death (which makes sense considering the role of vitamin C in collagen formation).

Some history of scurvy:

- Hippocrates was the first to describe the symptoms of scurvy in 400 BC.
- Incidence rapidly grew in the 14th and 15th c. as improved boat technology allowed for longer voyages. Entire crews were sometimes lost to scurvy with empty boats floating in the sea. For example, Magellan's fleet circled the world in 1519-1522 and lost 90% (!) of the crew to scurvy (this detail is often excluded from grade school lessons on explorers!).
- The first controlled clinical study recorded was for scurvy treatment. In 1747, James Lind treated men on his ship suffering from scurvy with either lemon juice, ale, seawater, vinegar, or dilute sulfuric acid. The men treated with the vitamin-C-rich lemon juice quickly recovered.
- Most animals can biosynthesize vitamin C, so there is no need to worry about dogs or cats with vitamin C deficiencies. Only a few species lack the required gene for biosynthesis, all primates (including humans) and guinea pigs.



*Answers to the in-class example:*

Identify the hybridization and geometry of each C atom:

- |  |  |
|--|--|
| C <sub>a</sub> : sp <sup>3</sup> (tetrahedral) | C <sub>d</sub> : sp <sup>2</sup> (trigonal planar) |
| C <sub>b</sub> : sp <sup>3</sup> (tetrahedral) | C <sub>e</sub> : sp <sup>2</sup> (trigonal planar) |
| C <sub>c</sub> : sp <sup>3</sup> (tetrahedral) | C <sub>f</sub> : sp <sup>2</sup> (trigonal planar) |

Identify the symmetry ( $\sigma$  or  $\pi$ ) and name the hybrid or atomic orbitals for each bond.

Bonds to carbon b:

- C<sub>b</sub>-H:  $\sigma$ (C2sp<sup>3</sup>, H1s)  
 C<sub>b</sub>-C<sub>a</sub>:  $\sigma$ (C2sp<sup>3</sup>, C2sp<sup>3</sup>)  
 C<sub>b</sub>-C<sub>c</sub>:  $\sigma$ (C2sp<sup>3</sup>, C2sp<sup>3</sup>)  
 C<sub>b</sub>-O:  $\sigma$ (C2sp<sup>3</sup>, O2sp<sup>3</sup>)

Bonds to carbon d:

- C<sub>d</sub>-O:  $\sigma$ (C2sp<sup>2</sup>, O2sp<sup>3</sup>)  
 C<sub>d</sub>-C<sub>c</sub>:  $\sigma$ (C2sp<sup>2</sup>, C2sp<sup>3</sup>)  
 C<sub>d</sub>-C<sub>e</sub>:  $\sigma$ (C2sp<sup>2</sup>, O2sp<sup>2</sup>)  
 $\pi$ (C2p<sub>x</sub>, O2p<sub>x</sub>) or  $\pi$ (C2p<sub>y</sub>, O2p<sub>y</sub>)

## Glucose Oxidation: Harnessing Energy from Plants

See page 3 and 4 of lecture 16 notes for the use of mean bond enthalpies to calculate the overall reaction enthalpy of glucose oxidation.

For the oxidation of glucose:



$\Delta H^\circ$  is negative - **exothermic**

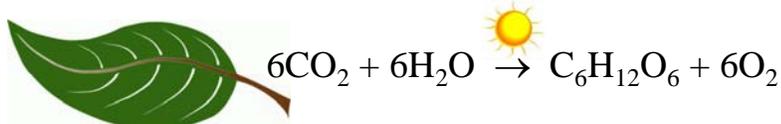
**Example 2) from page 3 of lecture 16 notes**

### *The oxidation of glucose*

**Plants convert carbon dioxide and water into sugar (glucose) and oxygen.**

\* This process requires energy.

\* We eat plants to get the energy stored in the glucose molecules.



**We perform the reverse reaction, the oxidation of glucose, to harness the stored energy.**



We store this energy in the form of ATP.