Hybridization of Atomic Orbitals

(Chapter 1 in the Klein text)
Basic Ideas

The atomic structures, from the Periodic Table, of atoms such as C, N, and O do not adequately explain how these atoms use orbitals to form bonds.

A hybridization model has therefore been developed in order to explain real structures, for example how all of the bond lengths and angles are equivalent in CH$_4$ (methane).
Why do we need this idea?

Consider water:

Facts: O-H bond lengths are equivalent; lone pairs are equivalent
Looking at the atoms that make H$_2$O

Each H atom has a single electron and is $1s^1$

The O atom has 8 total electrons and is $1s^2 2s^2 2px^2 2py^1 2pz^1$

The two lone pairs on O ($2s^2$ and $2px^2$) here are not the same but they are equivalent in H$_2$O, therefore we cannot use this atomic structure of O to make water – we have to modify it
Manipulating the Atomic Orbitals on O

We can translate the electronic structure to make it easier to see.

\[
\text{O} = 1s^2 \ 2s^2 \ 2px^2 \ 2py^1 \ 2pz^1
\]
The Hybridization Model for O

The lone pairs are not the same here so we need to modify the ground state picture to better match how O bonds in H₂O:

![Diagram showing energy levels and orbitals for O]
Building the Model

The blue horizontal lines represent the orbitals and the red arrows are the electrons occupying these orbitals.
Building the $sp^3$ Model

Here we manipulate by mixing (hybridizing) the $s$ and $p$ orbitals from the ground state configuration to give four $sp^3$ orbitals:
The $sp^3$ Model

Some things to notice about $sp^3$ orbitals:

- They are equivalent in size, shape, and energy.
- They are each $1/4$ s-like and $1/4$ p-like and will look somewhere in between these shapes.
Populating the Orbitals

We now have two equivalent lone pairs (sp³) and two half-filled orbitals (sp³) that will make sigma bonds with H atoms in H₂O.
The sp\(^3\) model in H\(_2\)O

Remember that these are atomic orbitals on O and that they must overlap with 1s orbitals from H to give H\(_2\)O.
Hybrid orbital patterns

There are only three orbital patterns that you need to know in the Organic Chemistry sequence.
The $sp^3$ picture for C, N and O

If there are no pi bonds, $sp^3$ hybrid orbitals are used
The sp³ picture for Carbon

The four sp³ orbitals from C project to the four corners of a regular tetrahedron.
Examples of sp$^3$ hybrid atoms

As examples, each of the C, N and O atoms in these molecules are sp$^3$ hybridized – all single bonds!
Orbitals of $sp^2$ hybrid atoms

The $sp^2$ picture has to accommodate a π bond by leaving one p orbital unchanged.
Hybrid orbitals contribute to sigma bonds

Notice that the hybrid \((sp^2)\) orbitals go to make single (sigma) bonds and the left over \(p\) orbital goes to the pi bond.
Overlap of sp$^2$ hybrid atoms

Two sp$^2$ hybrid C atoms overlap in ethylene, H$_2$C=CH$_2$
Examples of sp² hybrid atoms

As examples, each of the highlighted C, N and O atoms in these molecules are sp² hybridized – 1 pi bond!
The sp hybrid picture

When two pi bonds are formed by a C or N atom, sp hybrid orbitals are used.
The sp hybrid orbitals : sigma bonds

Notice that the hybrid (sp) orbitals go to make single (sigma) bonds and the left over p orbitals go to the pi bonds
The sp hybrid orbitals : alkynes

Notice that the hybrid (sp) orbitals go to make single (sigma) bonds and the left over p orbitals go to the pi bonds.
Examples of sp hybrid atoms

As examples, each of the highlighted C, N and atoms in these molecules are sp hybridized – 2 pi bonds!
Examples of hybridization: 1

Which atom and hybridization pattern does this picture represent?

- A) $sp^3$ O
- B) $sp^2$ N
- C) sp N
- D) $sp^3$ C
- E) sp C
Examples of hybridization: 1 answer

Which atom and hybridization pattern does this picture represent?

- A) sp^3 O
- B) sp^2 N
- C) sp N
- D) sp^3 C
- E) sp C

sp^2 hybrid Nitrogen
Examples of hybridization: 2

Which atom and hybridization pattern does this picture represent?

- A) $sp^3$ N
- B) $sp^2$ O
- C) $sp$ C
- D) $sp^2$ N
- E) $sp^3$ C
Examples of hybridization : 2 answer

Which atom and hybridization pattern does this picture represent?

- A) sp³ N
- B) sp² O
- C) sp C
- D) sp² N
- E) sp³ C

sp hybrid Carbon
Examples of hybridization : 3

Which atom and hybridization pattern does this picture represent?

- A) $sp\ C$
- B) $sp^2\ N$
- C) $sp^3\ C$
- D) $sp^3\ O$
- E) $sp^3\ N$
Examples of hybridization: 3 answer

Which atom and hybridization pattern does this picture represent?

- A) sp C
- B) sp$^2$ N
- C) sp$^3$ C
- D) sp$^3$ O
- E) sp$^3$ N

sp$^3$ hybrid Oxygen
Examples of hybridization : 4

Indicate the sp hybrid atom in the following molecule
Examples of hybridization : 4 answer

Indicate the sp hybrid atom in the following molecule
Examples of hybridization: 5

Indicate the sp$^3$ hybrid atom in the following molecule.
Examples of hybridization: 5 answer

Indicate the $sp^3$ hybrid atom in the following molecule.
Examples of hybridization : 6

Indicate the $sp^2$ hybrid atoms in the following molecule.
Examples of hybridization: 6 answer

Indicate the sp\(^2\) hybrid atoms in the following molecule.
Hybridization models

You can now apply these patterns to any organic molecule