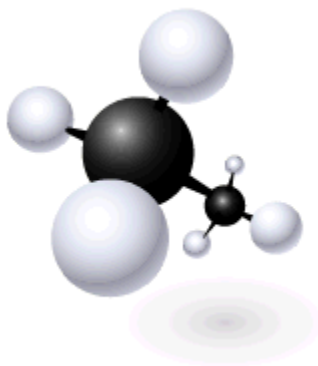


Hybridization of Atomic Orbitals

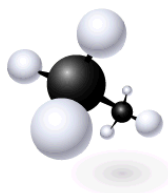
(Chapter 1 in the Klein text)



Basic Ideas

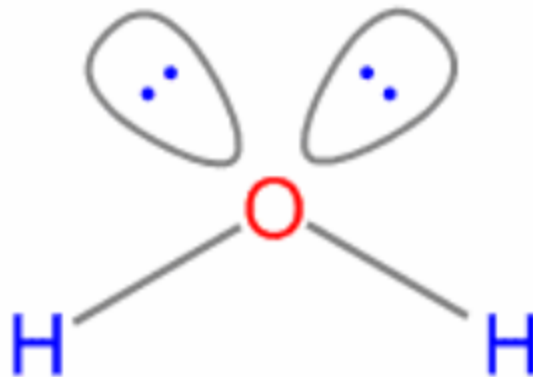
The atomic structures, from the Periodic Table, of atoms such as C, N, and O do not adequately explain how these atoms use orbitals to form bonds

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 CH₄ (methane)



Why do we need this idea?

Consider water:



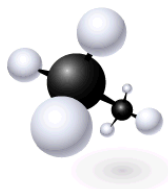
Facts: O-H bond lengths are equivalent; lone pairs are equivalent

Looking at the atoms that make H₂O

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

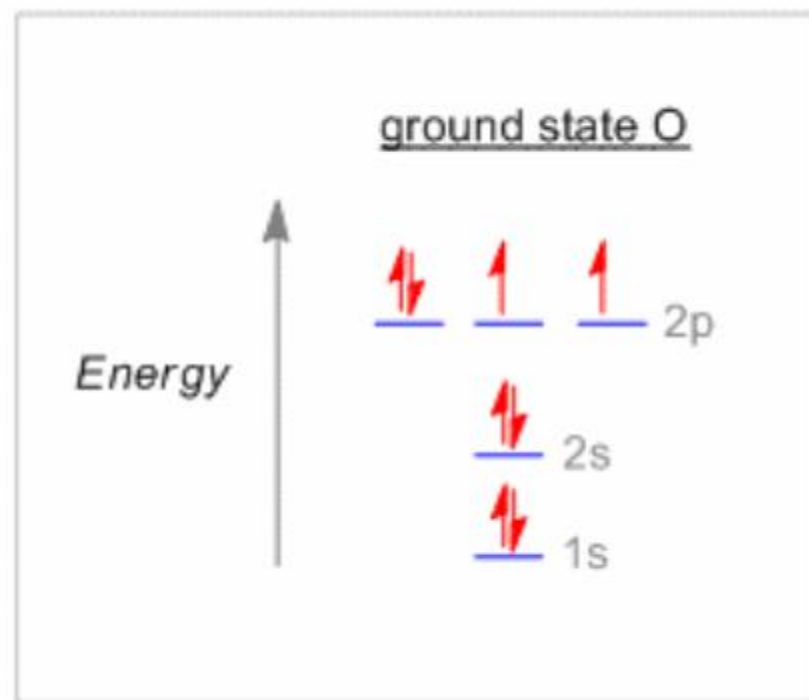
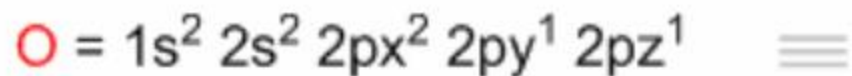
The O atom has 8 total electrons and is $1s^2 2s^2 2p_x^2 2p_y^1 2p_z^1$

The two lone pairs on O ($2s^2$ and $2p_x^2$) here are not the same but they are equivalent in H₂O, therefore we cannot use this atomic structure of O to make water – we have to modify it



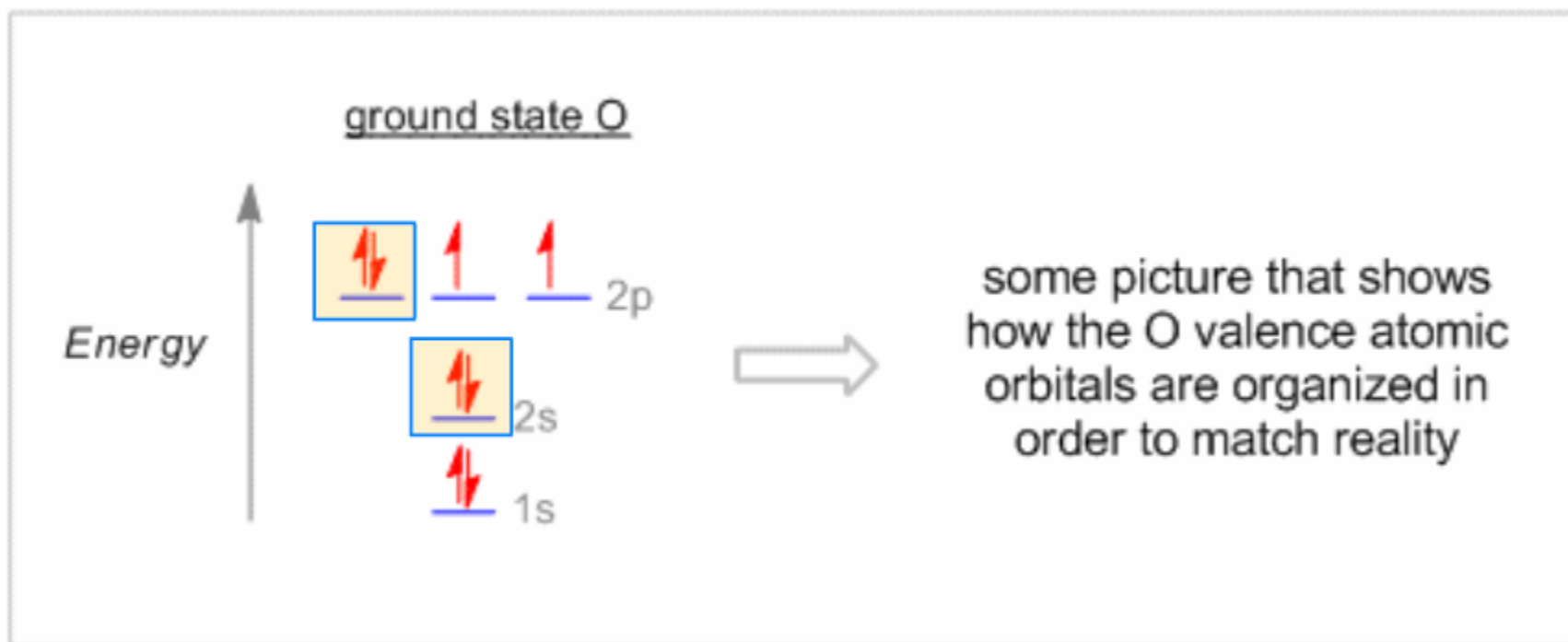
Manipulating the Atomic Orbitals on O

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



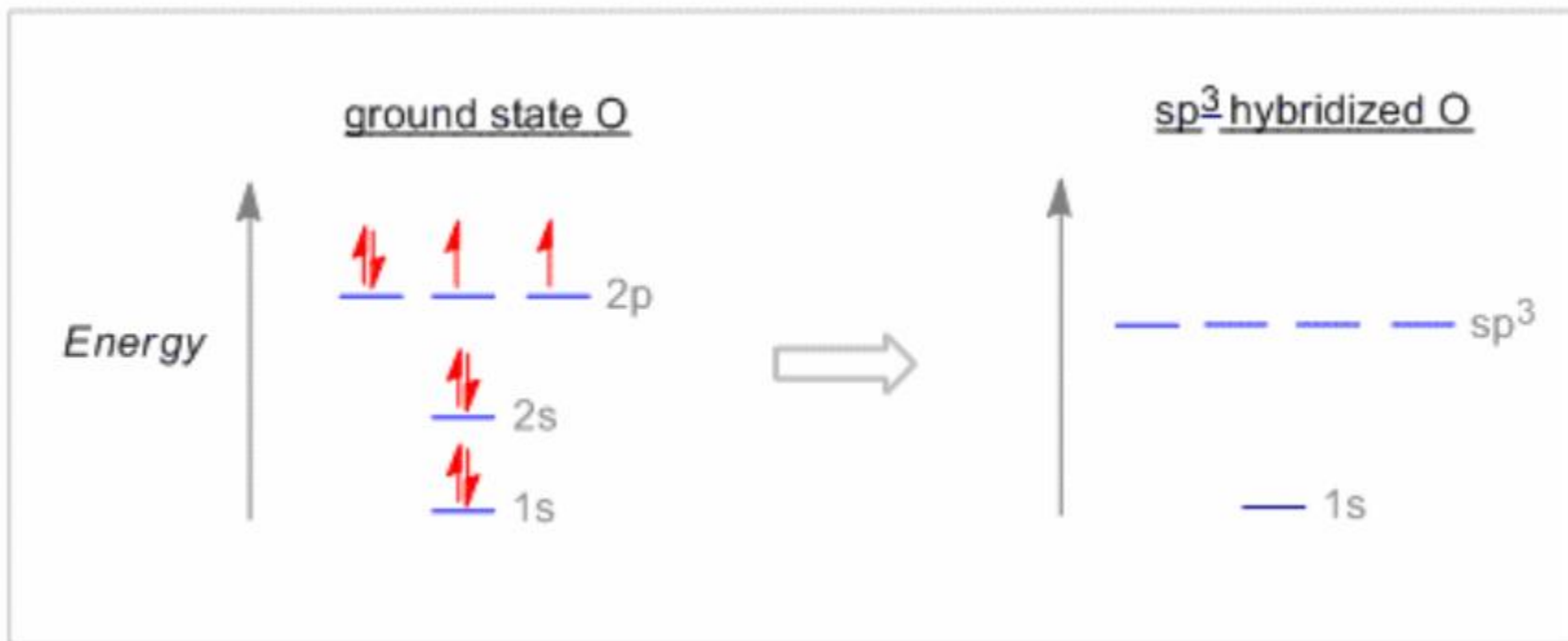
The Hybridization Model for O

The lone pairs are not the same here so we need to modify the ground state picture to better match how O bonds in H_2O :



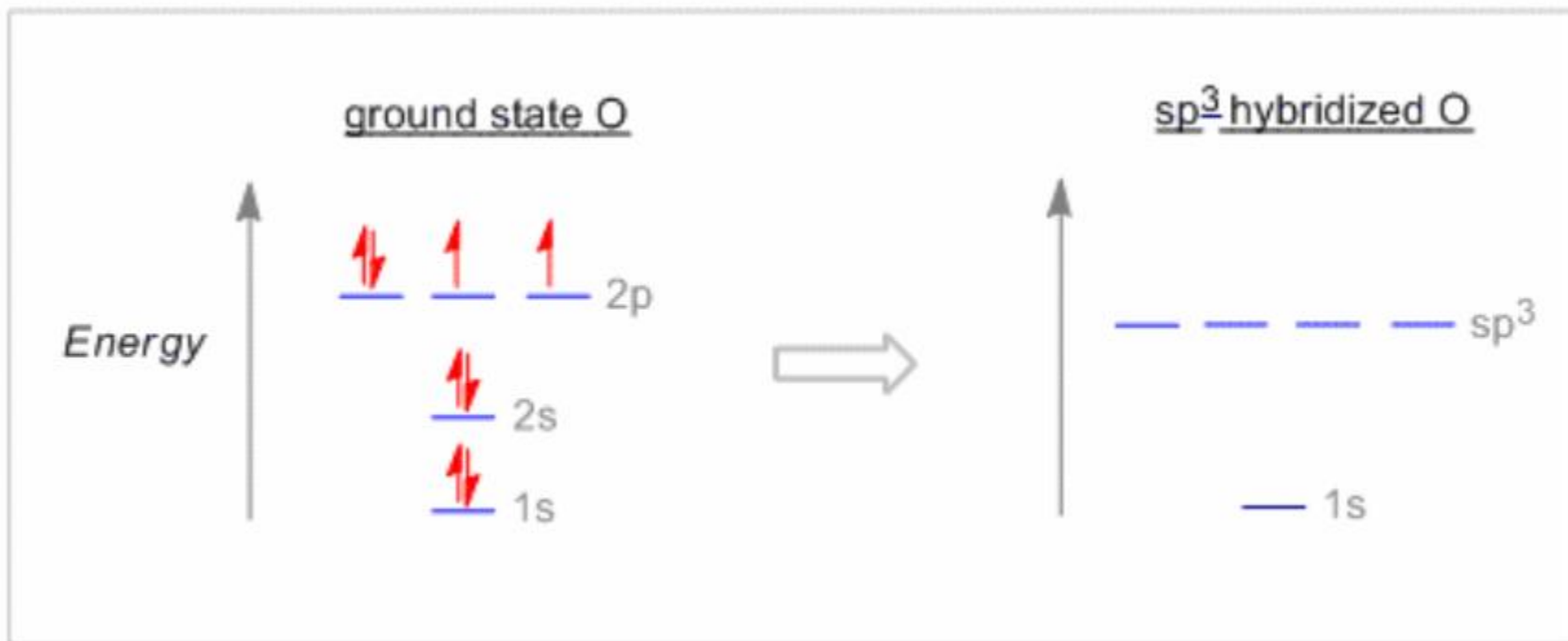
Building the Model

The blue horizontal lines represent the orbitals and the red arrows are the electrons occupying these orbitals



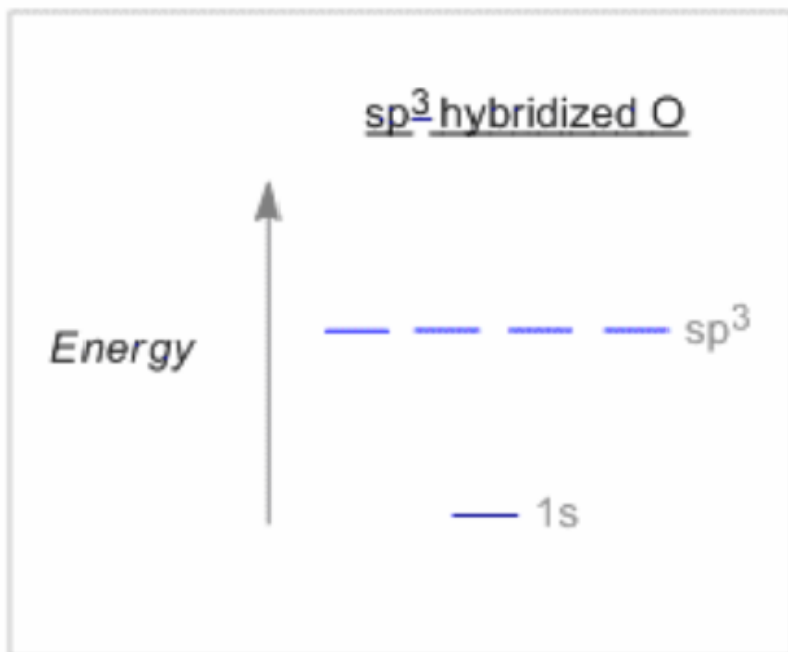
Building the sp^3 Model

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



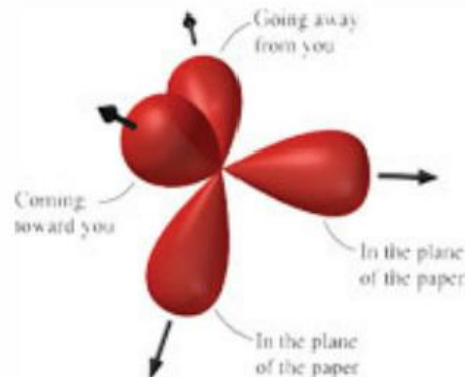
The sp^3 Model

Some things to notice about sp^3 orbitals:



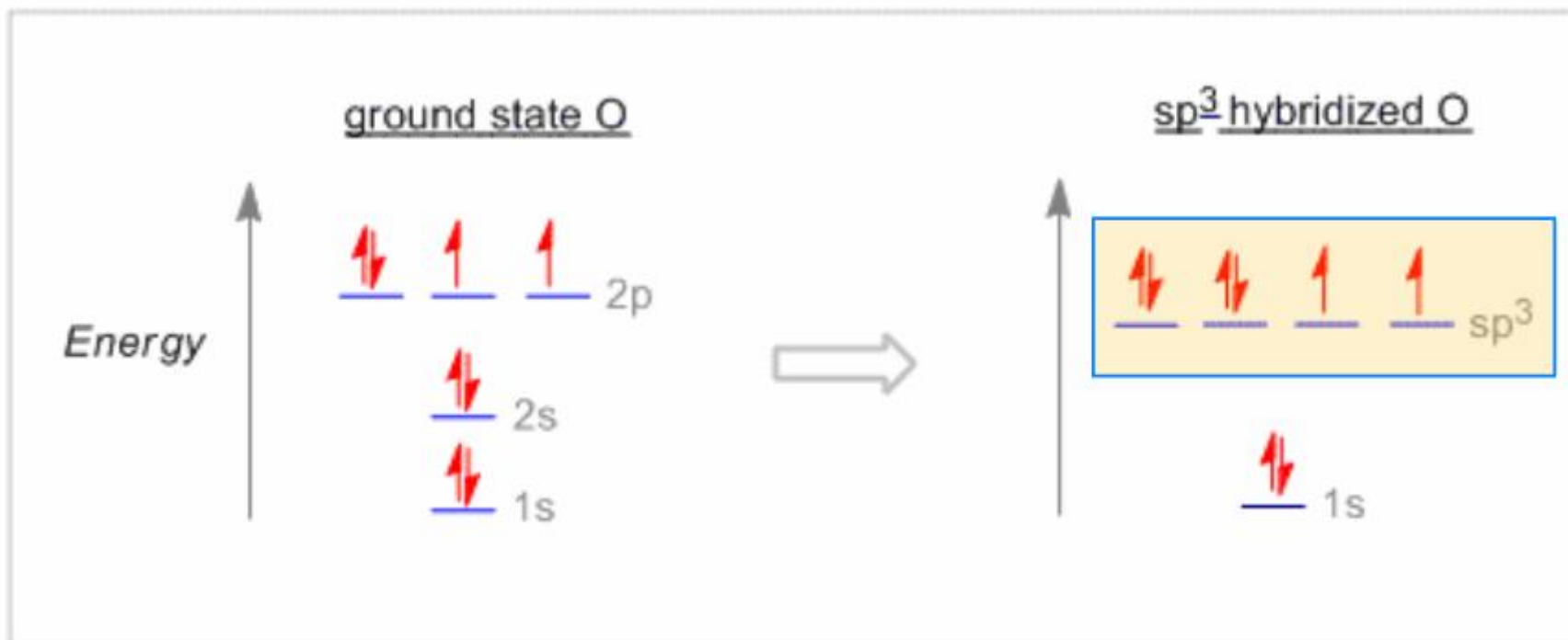
They are equivalent in size, shape, and energy

They are each 1/4 s-like and 1/4 p-like and will look somewhere in between these shapes



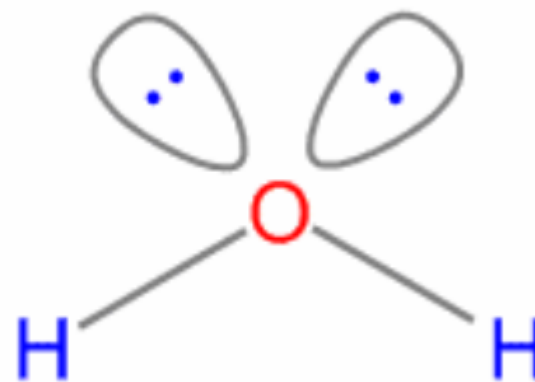
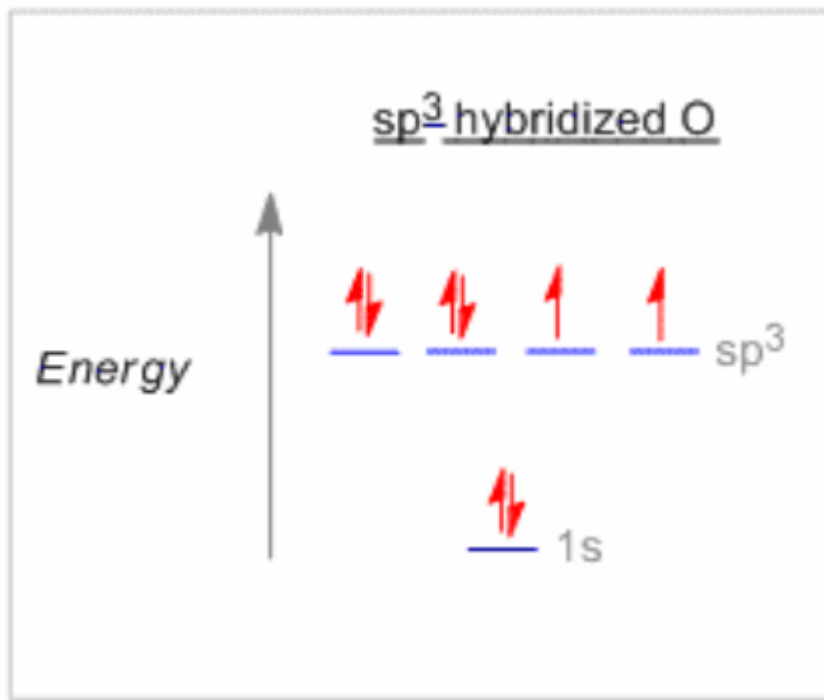
Populating the Orbitals

We now have two equivalent lone pairs (sp^3) and two half-filled orbitals (sp^3) that will make sigma bonds with H atoms in H_2O



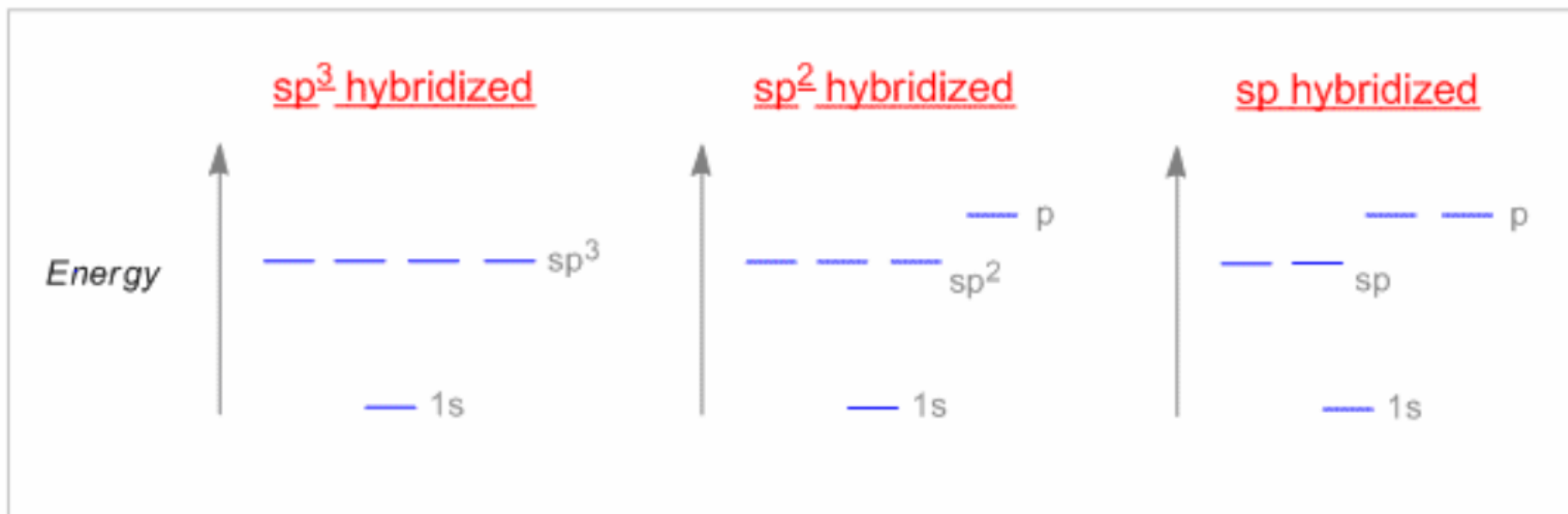
The sp^3 model in H_2O

Remember that these are **atomic orbitals** on O and that they must overlap with 1s orbitals from H to give H_2O



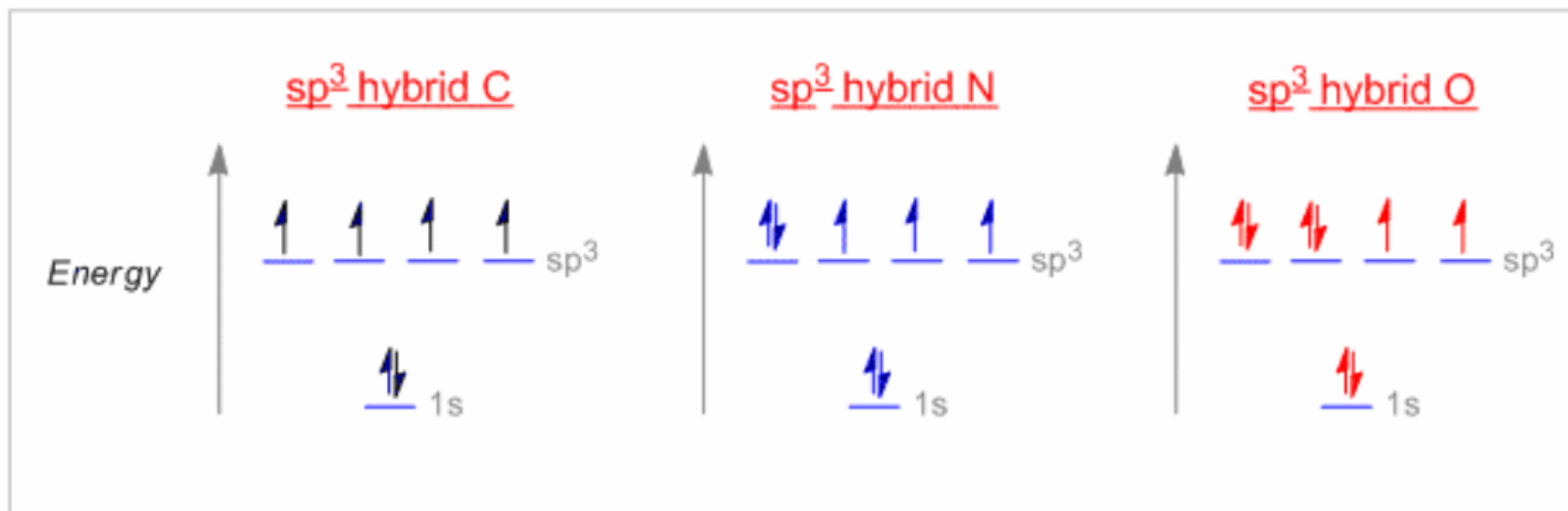
Hybrid orbital patterns

There are only three orbital patterns that you need to know in the Organic Chemistry sequence



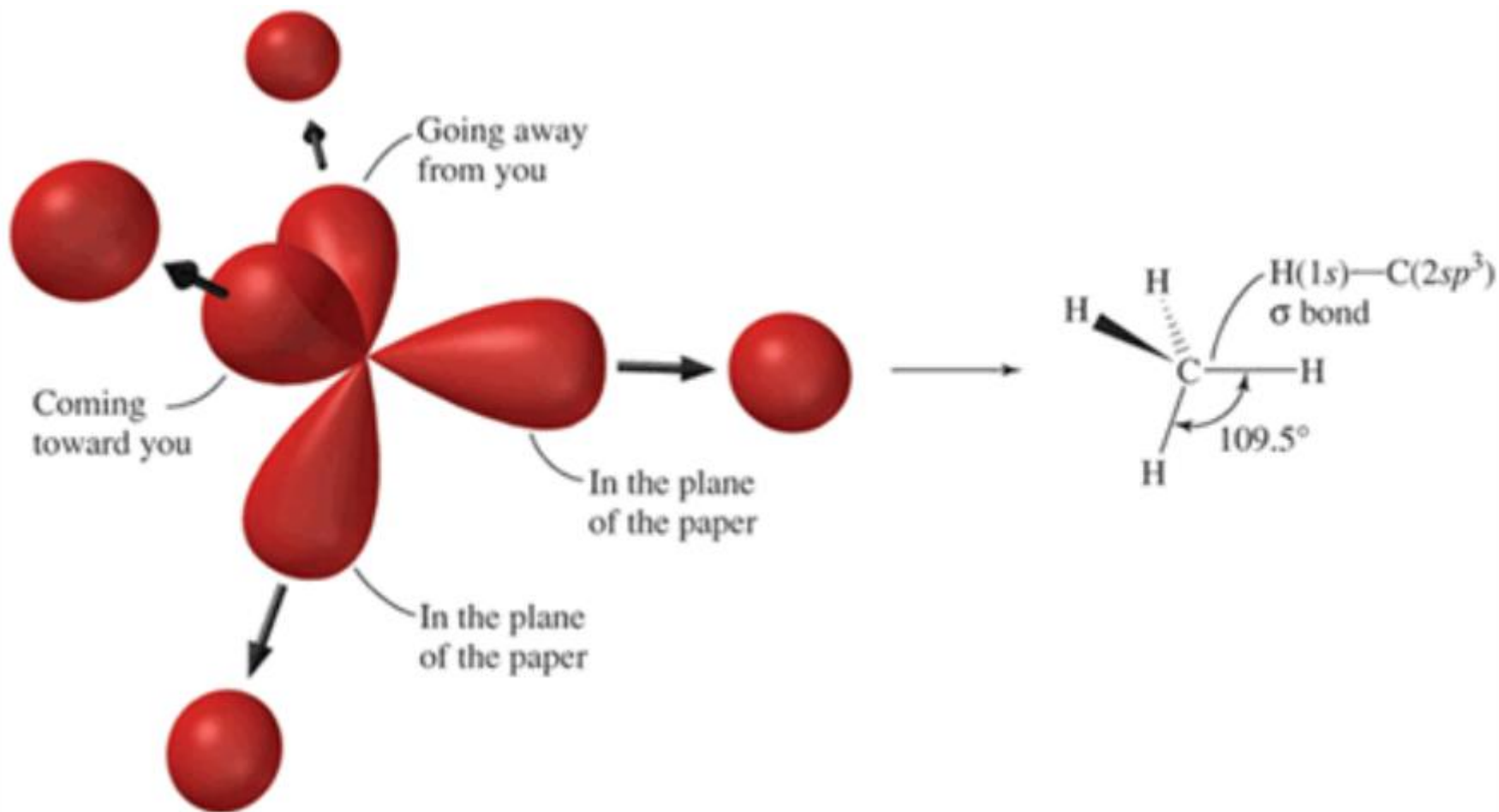
The sp^3 picture for C, N and O

If there are no pi bonds, sp^3 hybrid orbitals are used



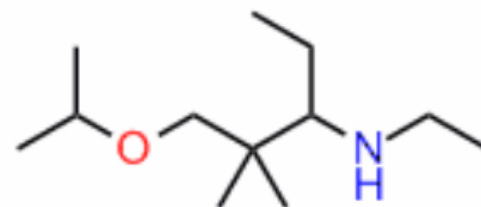
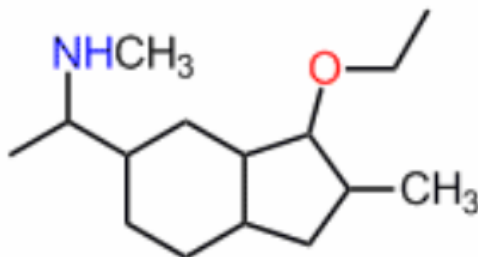
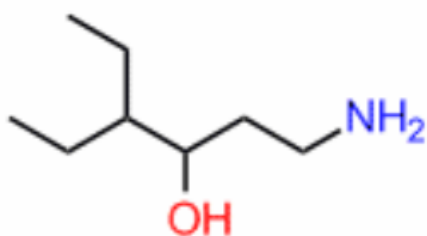
The sp^3 picture for Carbon

The four sp^3 orbitals from C project to the four corners of a regular tetrahedron



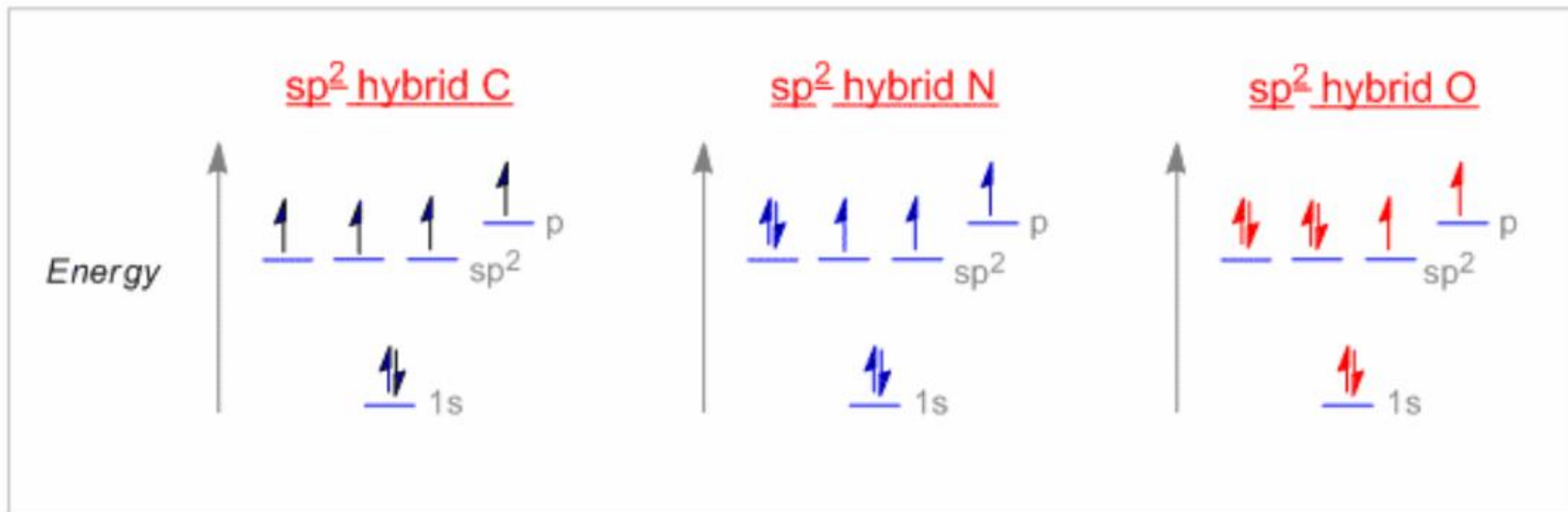
Examples of sp^3 hybrid atoms

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



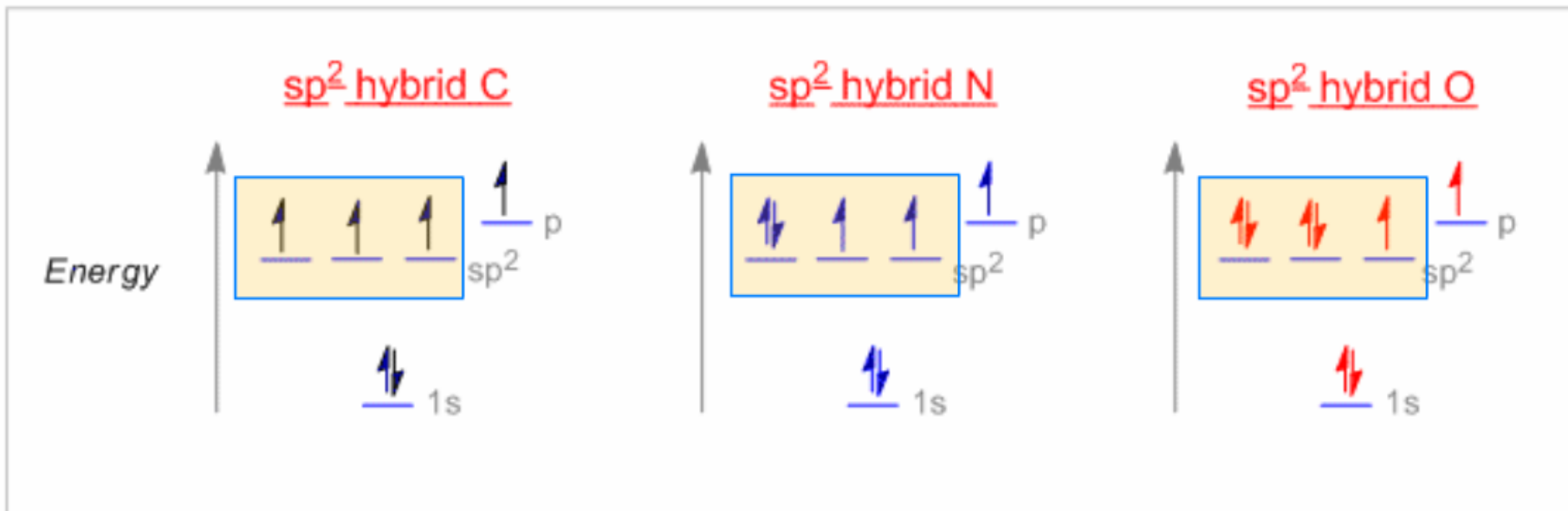
Orbitals of sp^2 hybrid atoms

The sp^2 picture has to accommodate a pi bond by leaving one p orbital unchanged



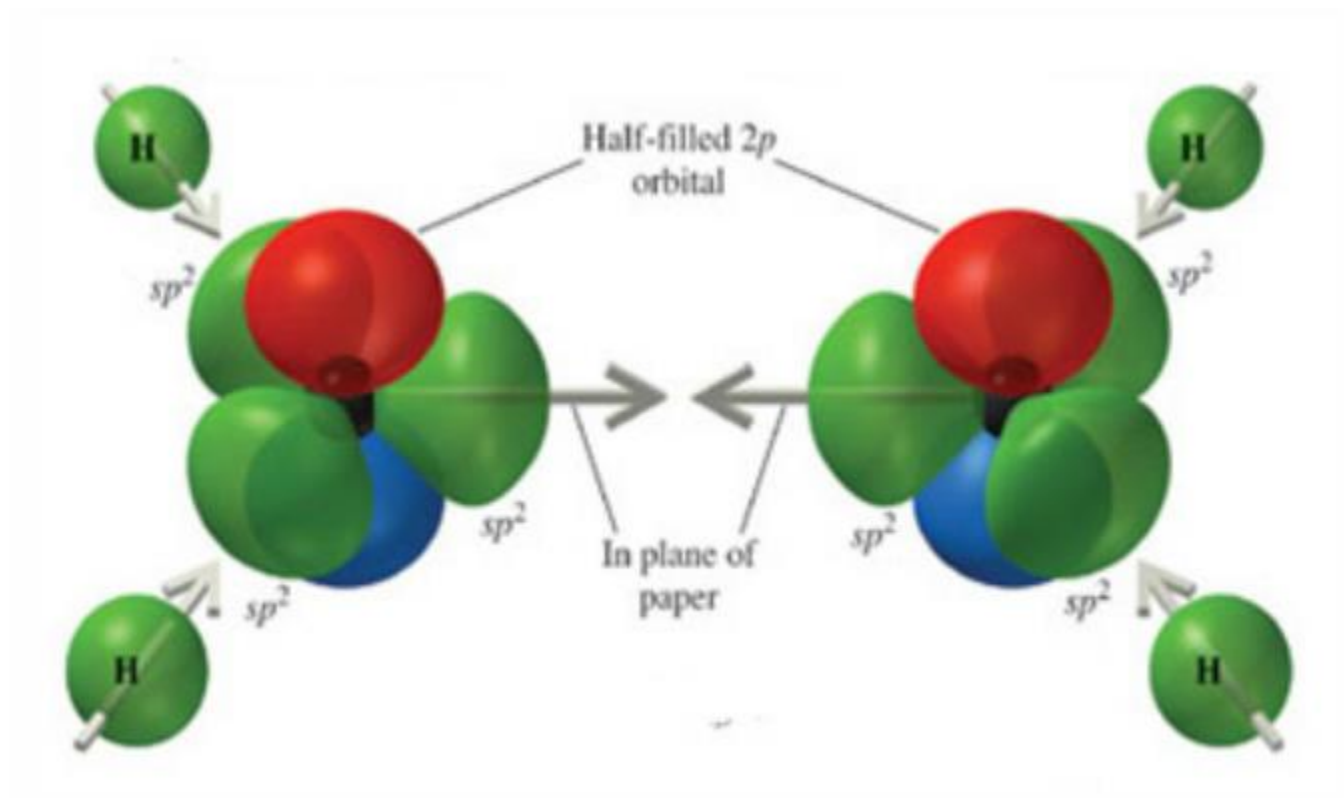
Hybrid orbitals contribute to sigma bonds

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



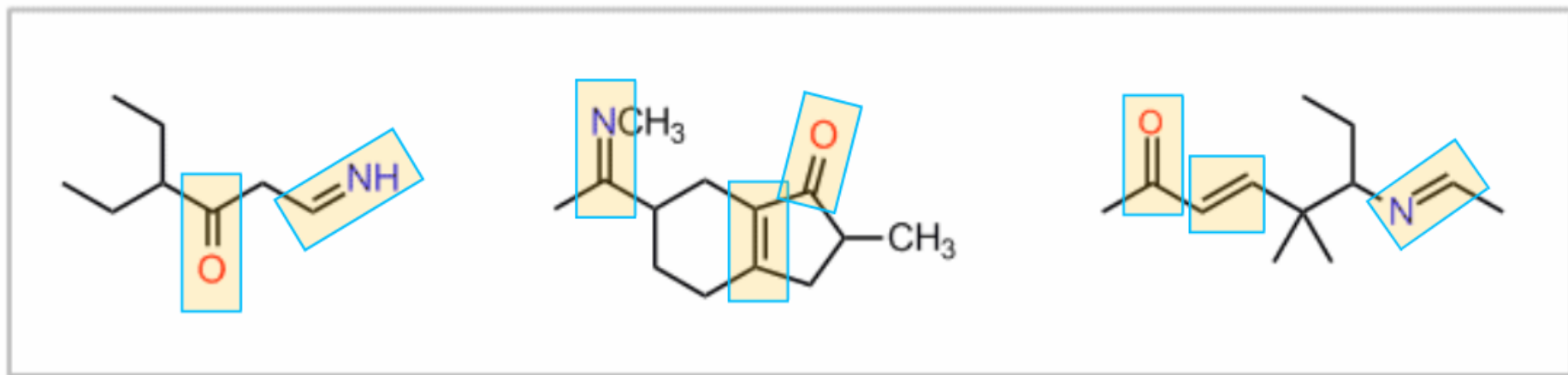
Overlap of sp^2 hybrid atoms

Two sp^2 hybrid C atoms overlap in ethylene, $\text{H}_2\text{C}=\text{CH}_2$



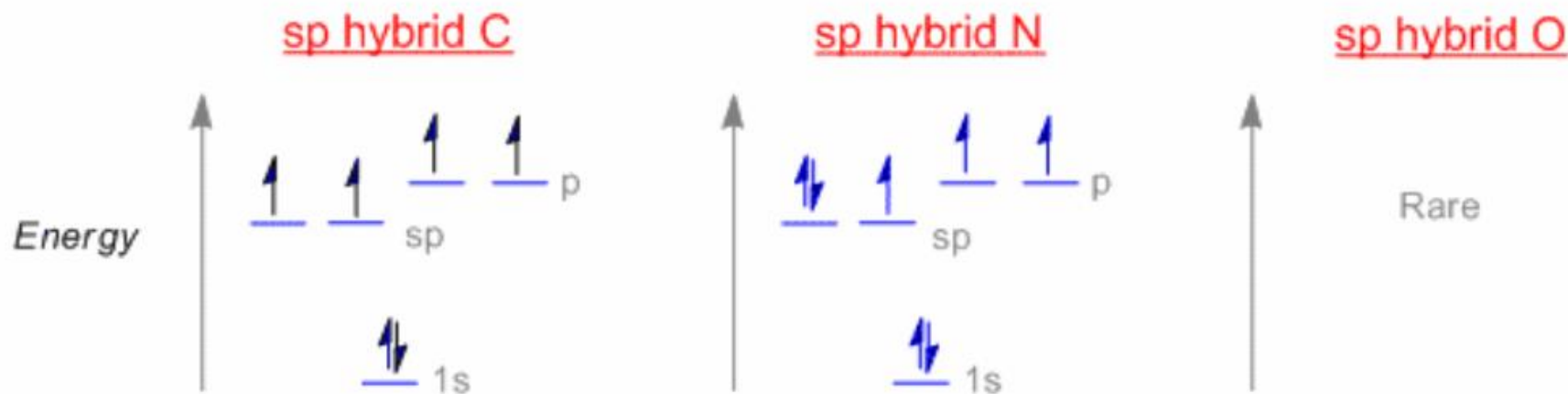
Examples of sp^2 hybrid atoms

As examples, each of the highlighted C, N and O atoms in these molecules are sp^2 hybridized – 1 pi bond!



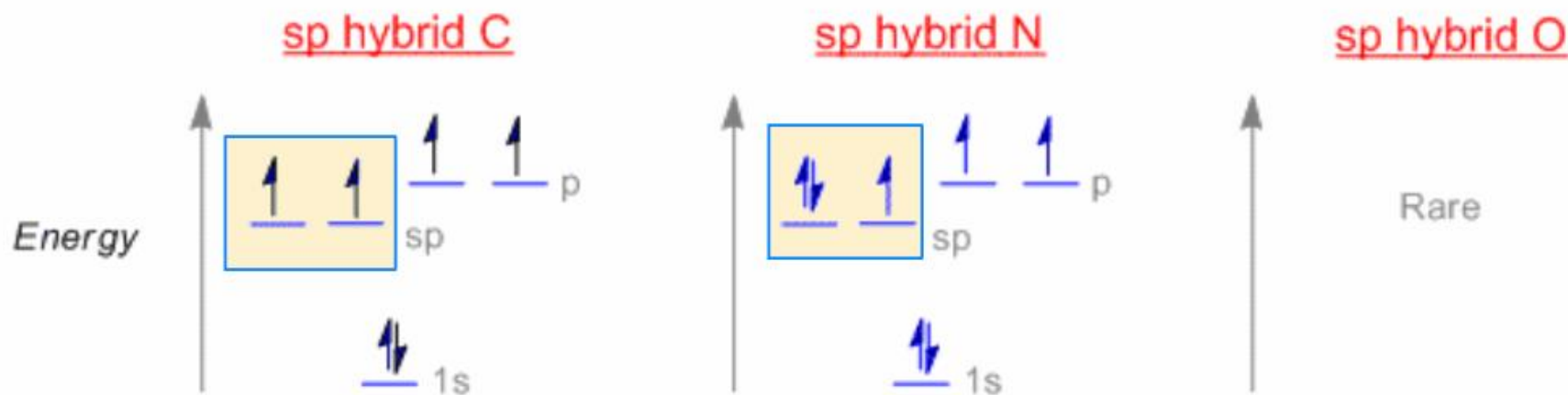
The sp hybrid picture

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



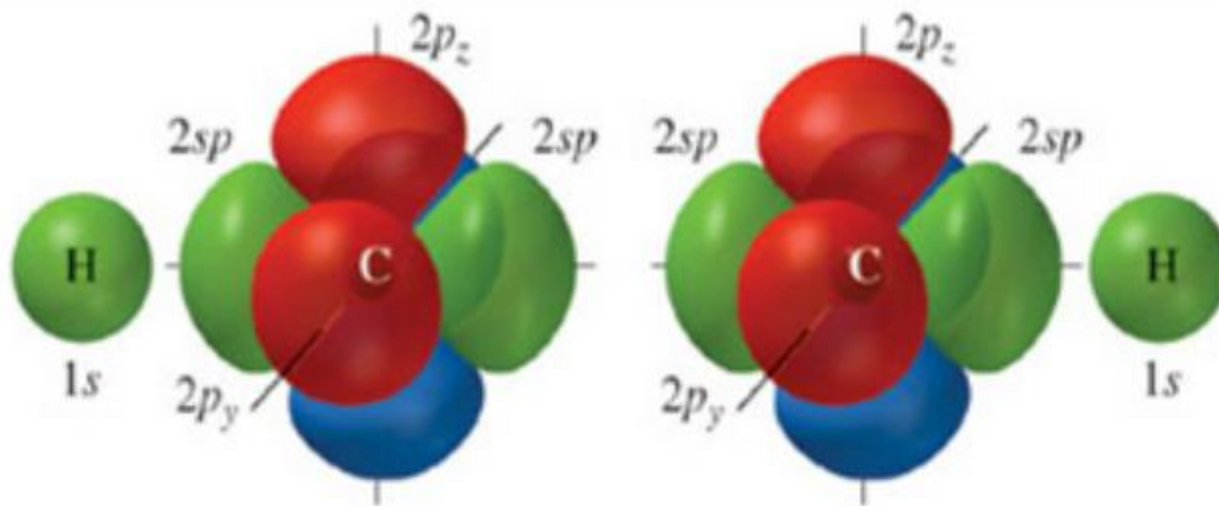
The sp hybrid orbitals : sigma bonds

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



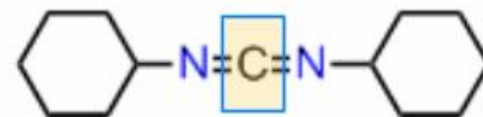
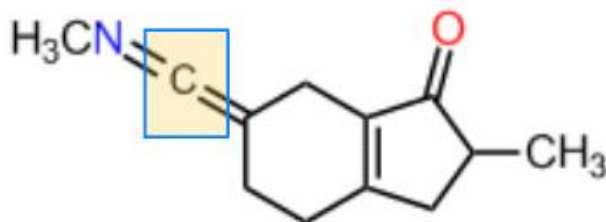
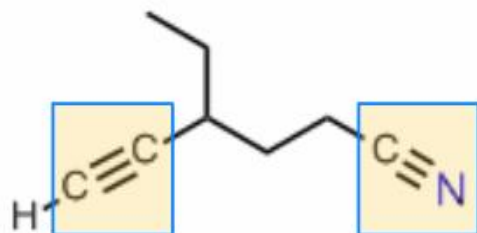
The sp hybrid orbitals : alkynes

Notice that the hybrid (sp) orbitals go to make single (sigma) bonds and the left over p orbitals go to the π bonds



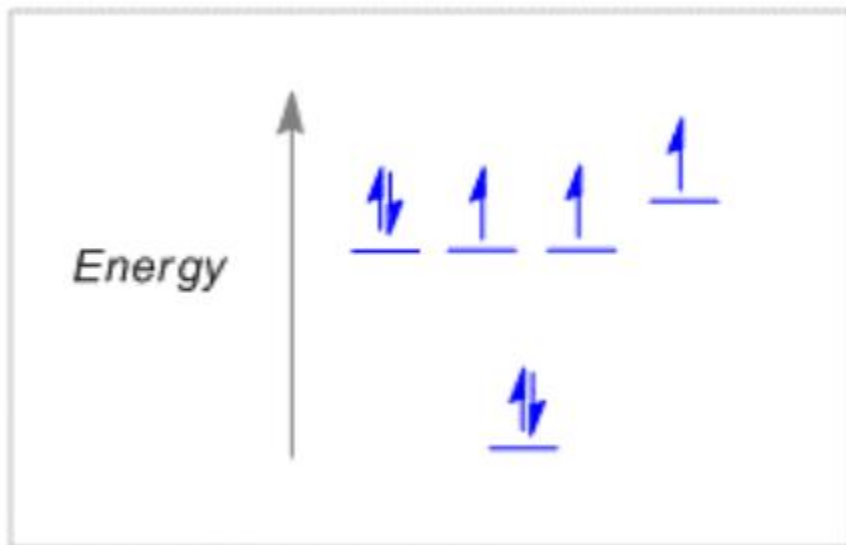
Examples of sp hybrid atoms

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



Examples of hybridization : 1

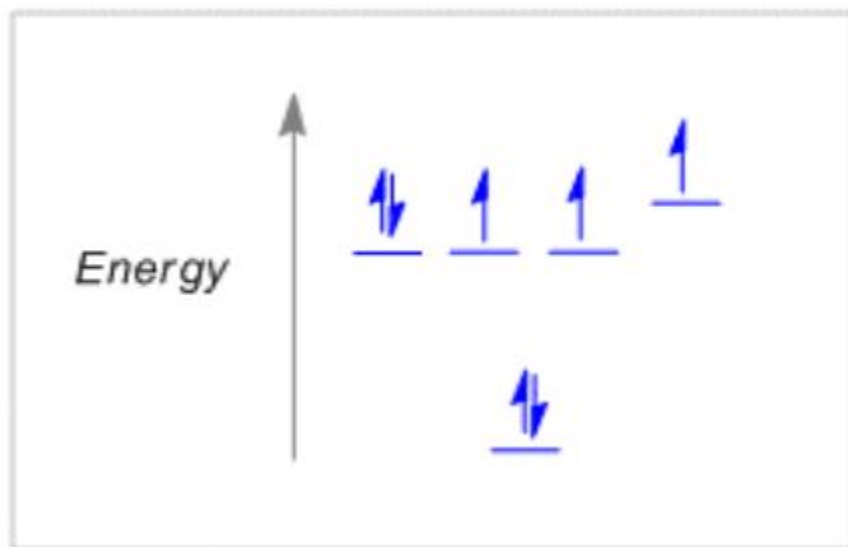
Which atom and hybridization pattern does this picture represent?



- ☐ 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?

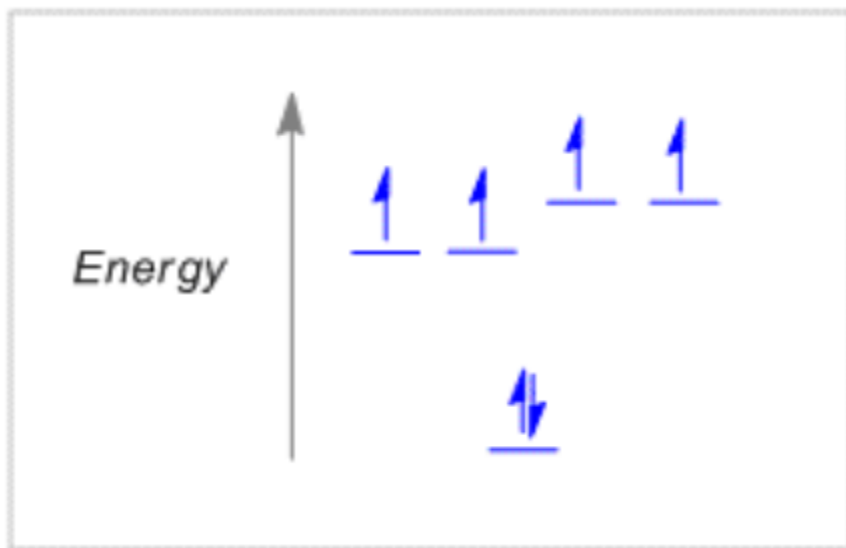


- ☐ A) sp^3 O
- ☐ B) sp^2 N
- ☐ C) sp N
- ☐ D) sp^3 C
- ☐ E) sp C

sp^2 hybrid Nitrogen

Examples of hybridization : 2

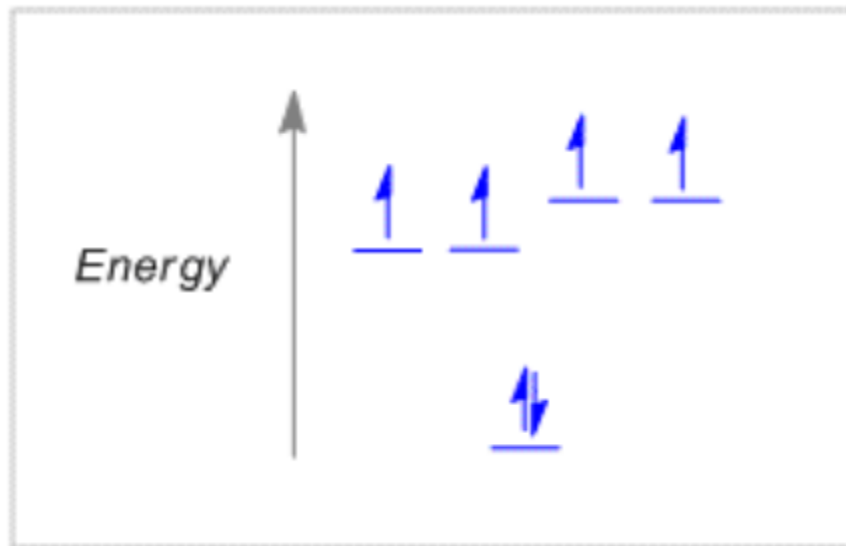
Which atom and hybridization pattern does this picture represent?



- ☐ 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?

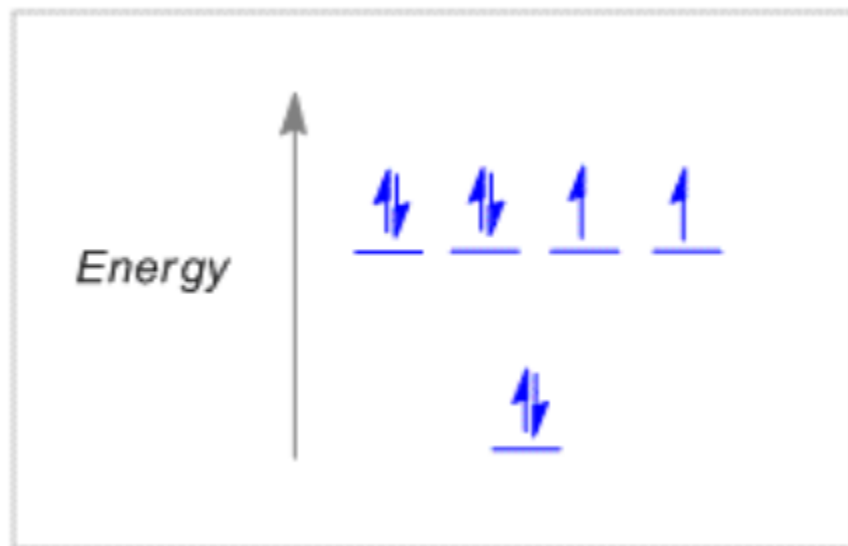


- ☐ A) sp^3 N
- ☐ B) sp^2 O
- ☐ C) sp C
- ☐ D) sp^2 N
- ☐ E) sp^3 C

sp hybrid Carbon

Examples of hybridization : 3

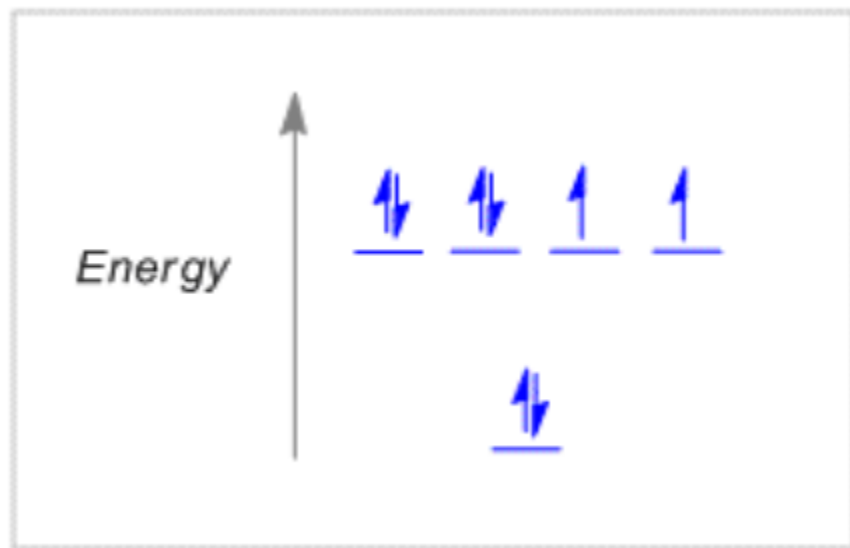
Which atom and hybridization pattern does this picture represent?



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

Examples of hybridization : 3 answer

Which atom and hybridization pattern does this picture represent?

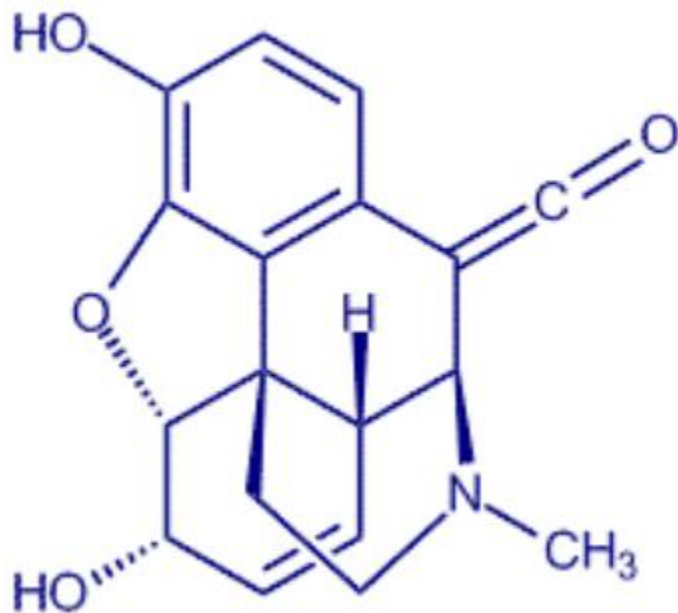


- ☐ A) sp C
- ☐ B) sp^2 N
- ☐ C) sp^3 C
- ☐ D) sp^3 O
- ☐ E) sp^3 N

sp^3 hybrid Oxygen

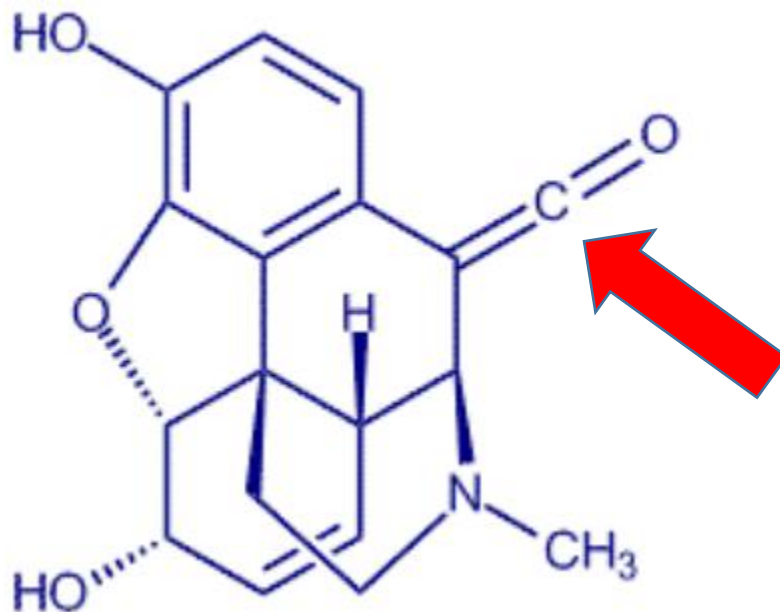
Examples of hybridization : 4

Indicate the sp hybrid atom in the following molecule



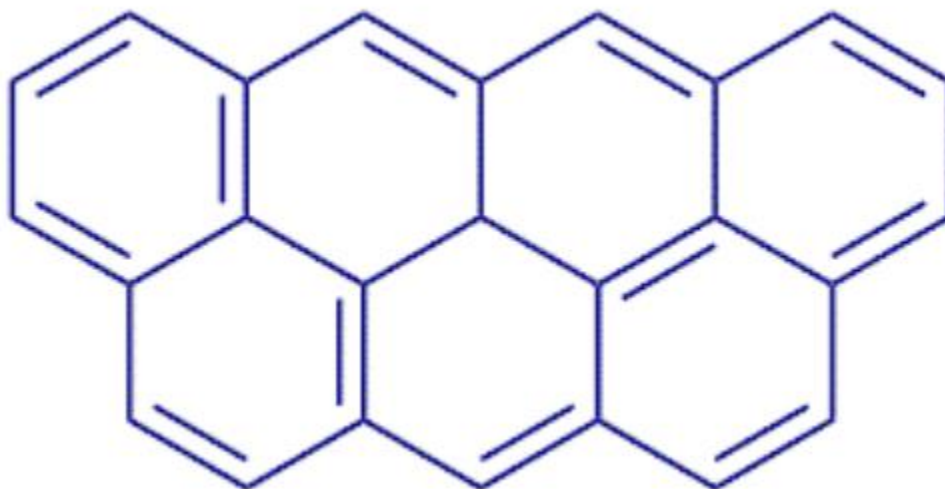
Examples of hybridization : 4 answer

Indicate the sp hybrid atom in the following molecule



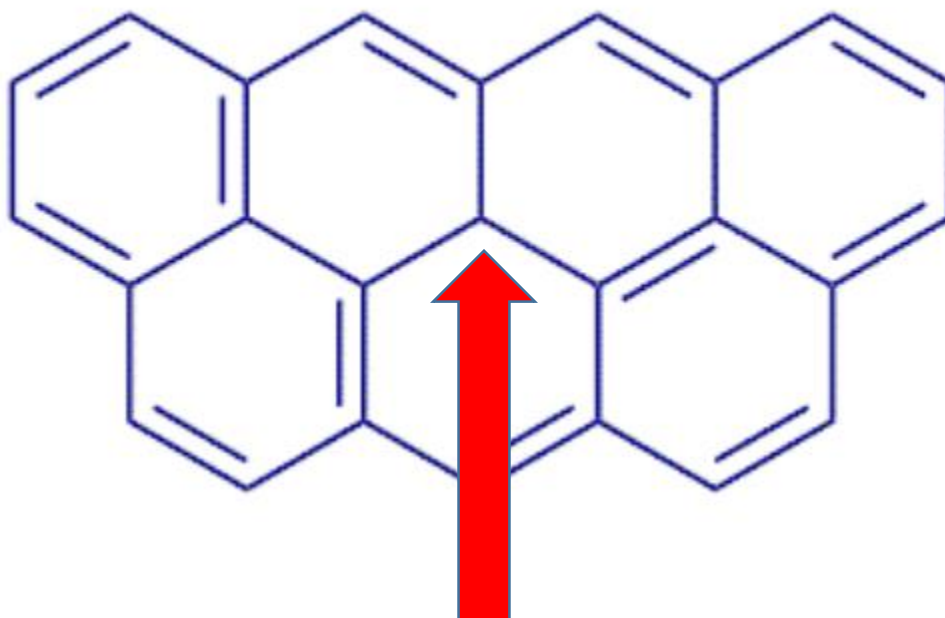
Examples of hybridization : 5

Indicate the sp^3 hybrid atom in the following molecule



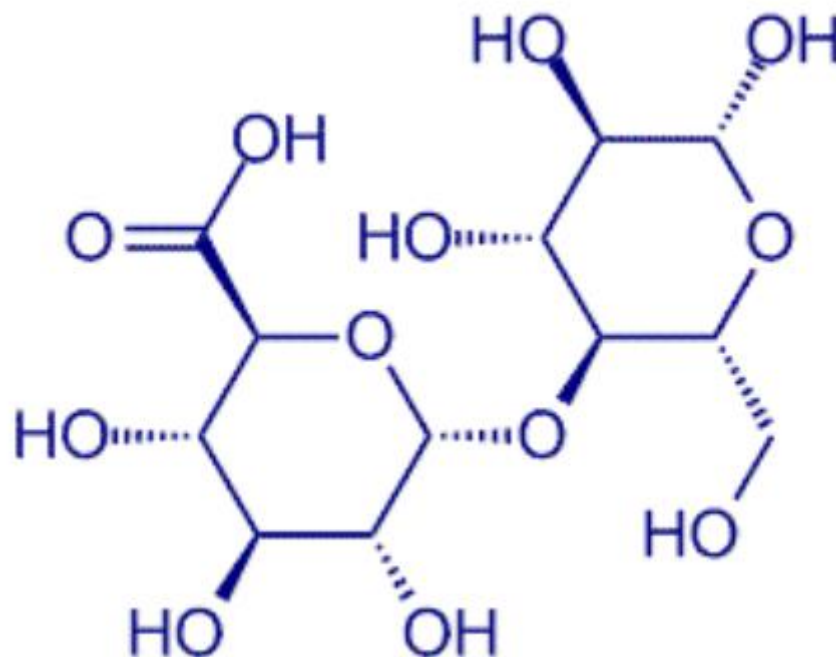
Examples of hybridization : 5 answer

Indicate the sp^3 hybrid atom in the following molecule



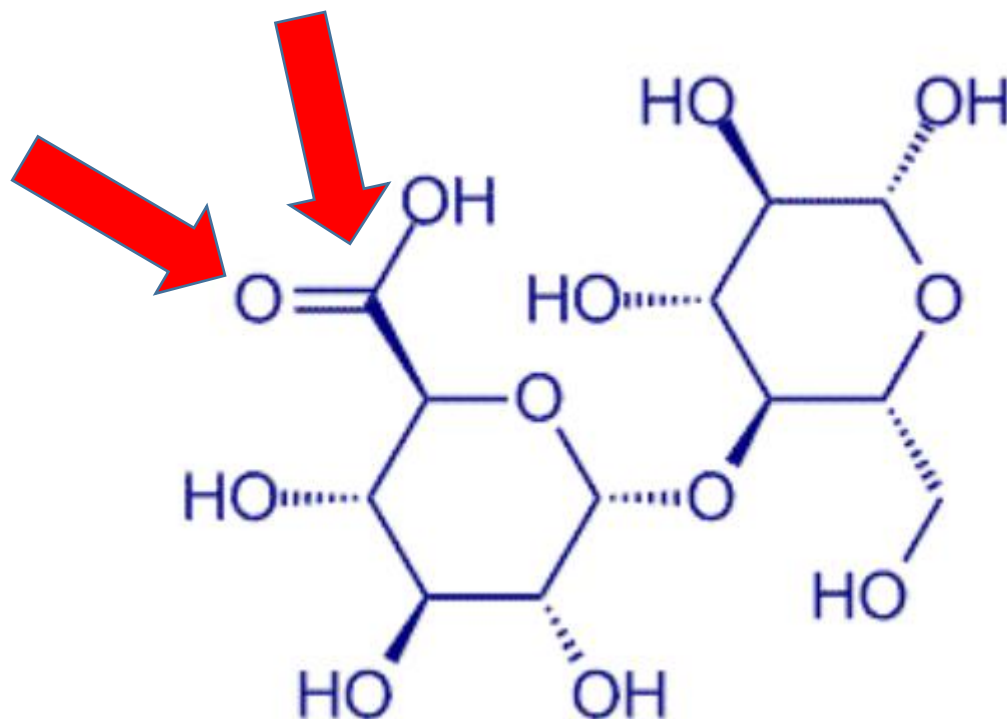
Examples of hybridization : 6

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

