Lewis Structures: NF_3

1. Determine the total number of valence electrons

2. Build an appropriate skeleton structure

3. Distribute remaining electrons as lone pairs to the most electronegative atoms first, completing octets

4. Share electrons with less electronegative atoms, turning lone pairs into bonds, to complete octets.

Exceptions to the Octet Rule

Atoms with fewer than 4 valence electrons (e.g. Be, B) can be satisfied with **less than an octet**.

e.g. BF_3:

Molecules with an **odd number of electrons** (radicals) cannot achieve an octet.

e.g. NO_2

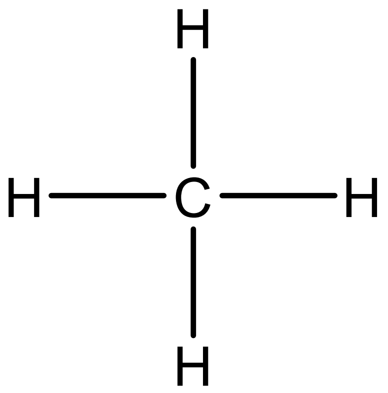
Atoms that have *n=3* or greater can have an **expanded octet** (typically 10 or 12 electrons on the central atom)

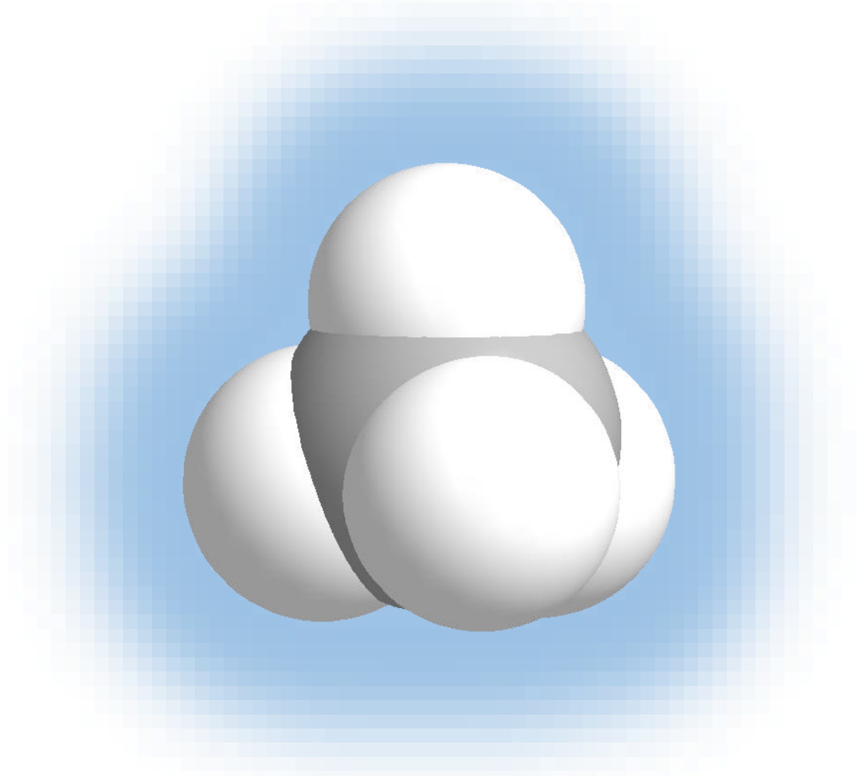
e.g. SF_6:

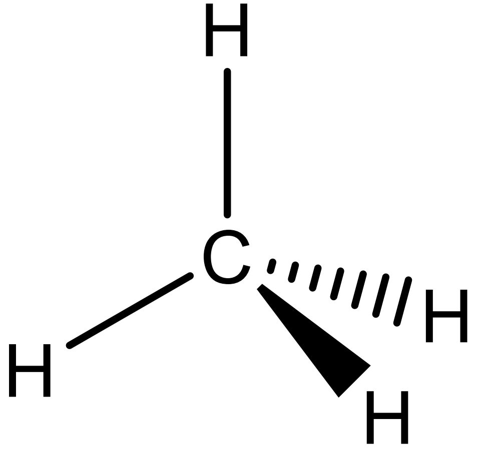
Draw Lewis Structures, determine bond polarity and order for:

XeF_2	SF_4	HOBr
BrF_5	BrF_3	HCCH
PF_5	$KrCl_4$	$CH_3C(O)(OH)$

Describing Shapes of Molecules: VSEPR







VSEPR Basics

Electrons are all negatively charged – so they will repel each other.

Bonds and “lone pairs” will be arranged around a central atom to be as far apart as possible and minimize repulsions. (*Multiple bonds (=, ≡) count as one “electron group”)*

TWO e^- groups around central atom

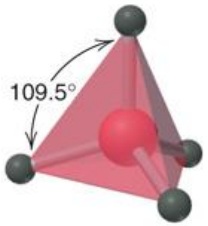
Linear

THREE e^- groups on central atom

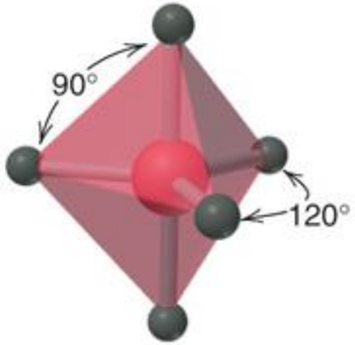
Trigonal planar

FOUR e^- groups on central atom

Tetrahedral



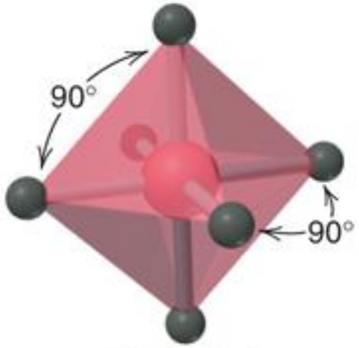
FIVE e$^-$ groups on central atom



Trigonal bipyramidal

Trigonal bipyramidal

SIX e$^-$ groups on central atom



Octahedral

Octahderal

https://phet.colorado.edu/sims/html/molecule-shapes-basics/latest/molecule-shapes-basics_en.html

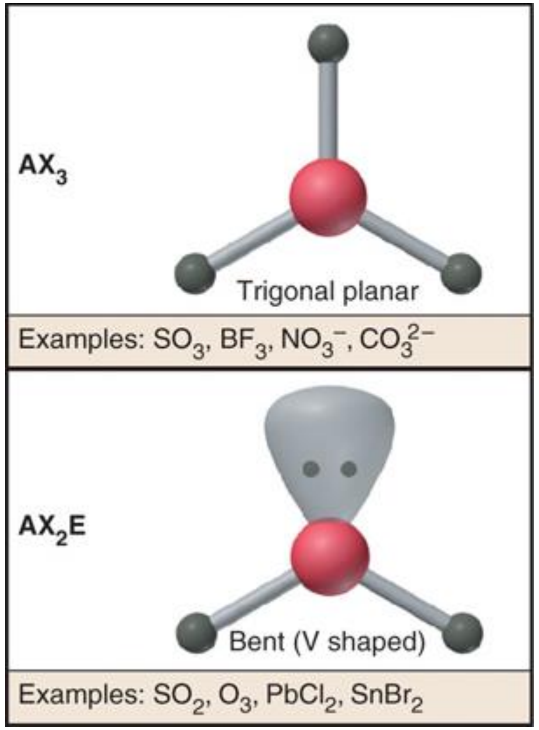
Electron-pair vs. Molecular Shapes

Electron-pair geometries count all electron groups around the central atom.

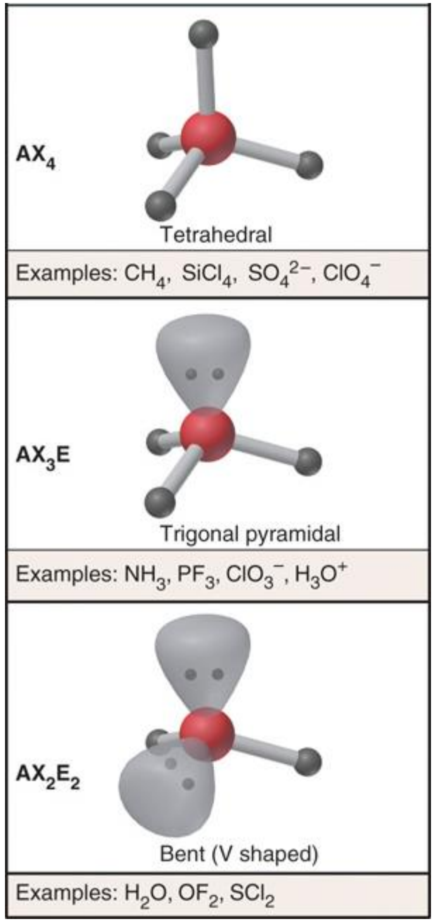
However, when observing molecules with many techniques, we only see the locations of the **atoms**, and lone pairs are essentially invisible.

Treating lone pairs as "invisible" but still contributing to the shape of the molecule gives the **molecular geometries.**

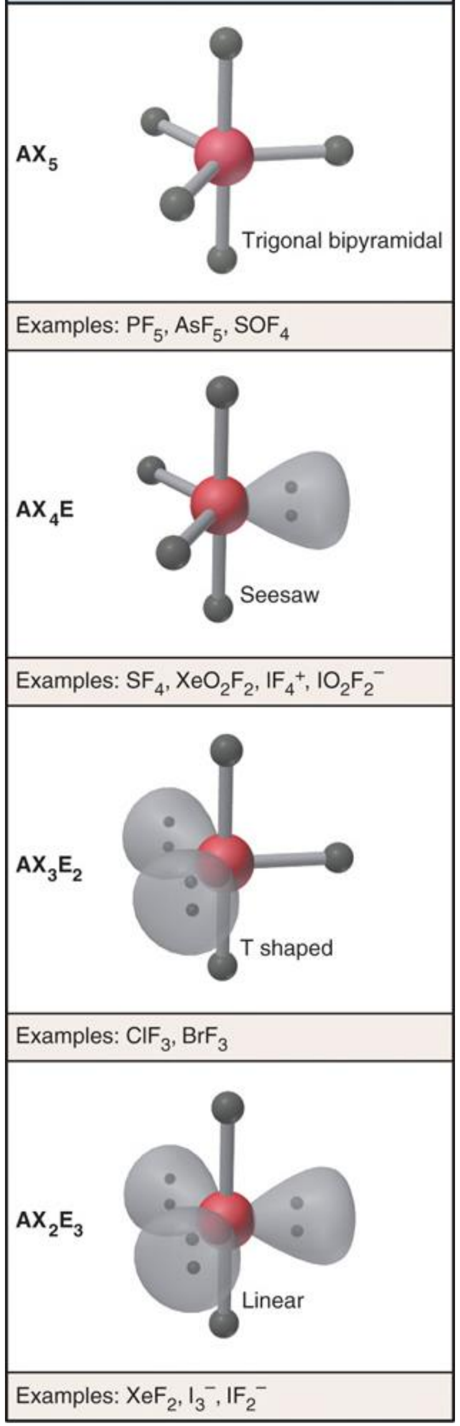
Based on
Trigonal planar
(3 electron groups)



Based on
Tetrahedral
(4 electron groups)



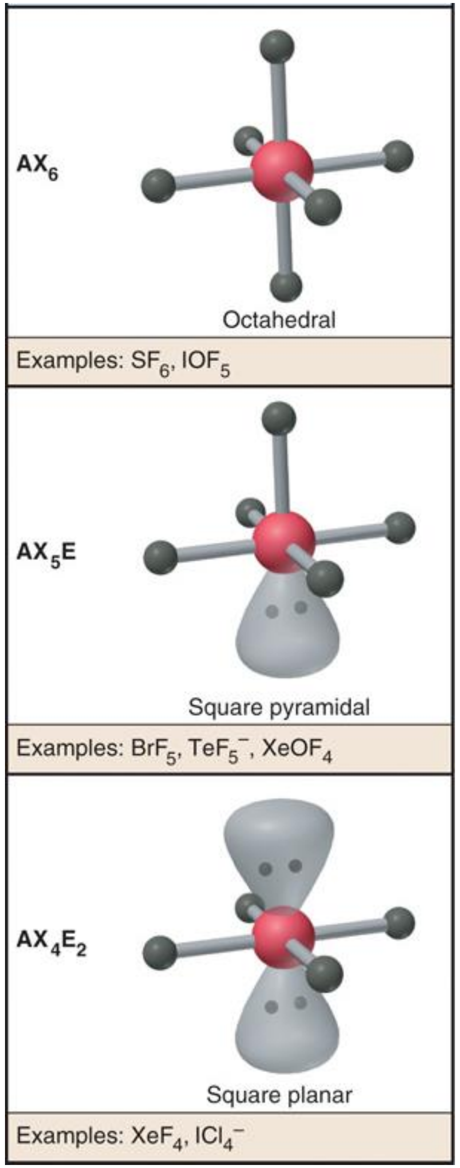
Based on
Trigonal bipyramidal
(5 electron groups)



Based on

Octahedral

(6 electron groups)



What is the molecular geometry of NF_3?

a. Linear

b. Trigonal planar

c. Tetrahedral

d. Trigonal bipyramidal

e. Octahedral

Molecular Polarity

We've seen that **bonds** can be polar or nonpolar. The combination of bonds and their arrangement around the central atom determines the **overall molecular polarity**.

e.g. CO_2

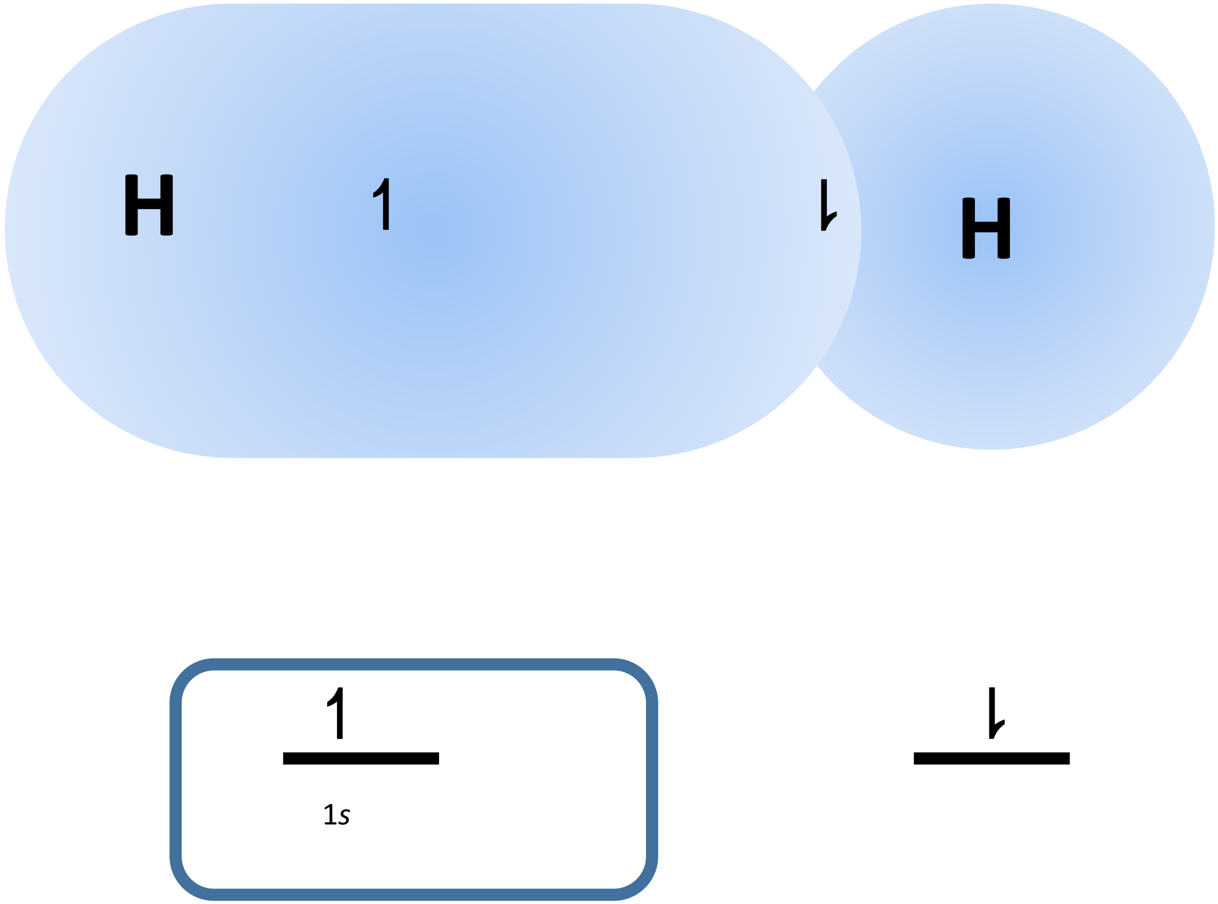
H_2O:

CCl_4:

$CHCl_{3:}$

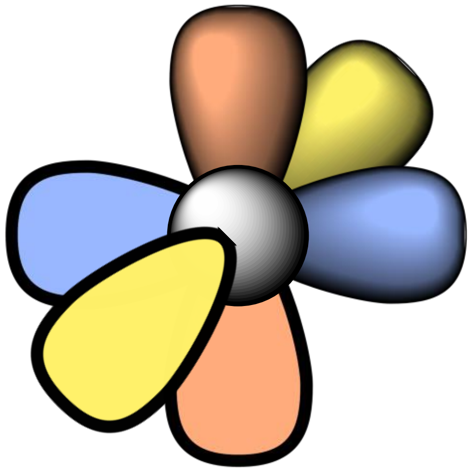
Valence Bond Theory

In **valence bond theory**, bonds are formed from the overlap of atomic orbitals (valence atomic orbitals). This overlap allows bonds to form and is the source of the 'sharing' in a covalent bond.



Methane?

So, based on VB theory, C in CH_4 should be using its 2*s* and 2*p* orbitals to form 4 bonds to H atoms (which are using their *1s* orbitals):

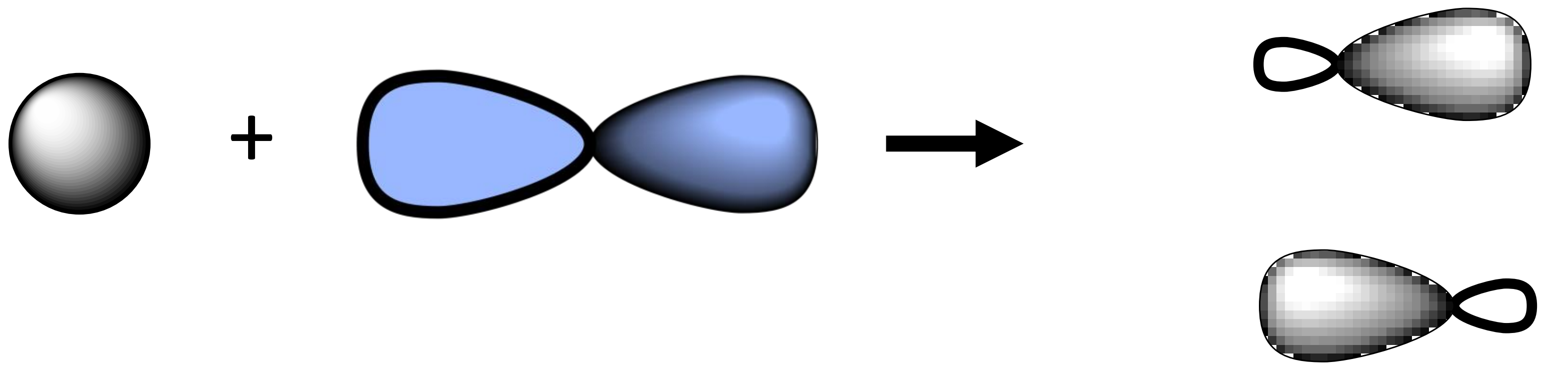


Hybrid orbitals

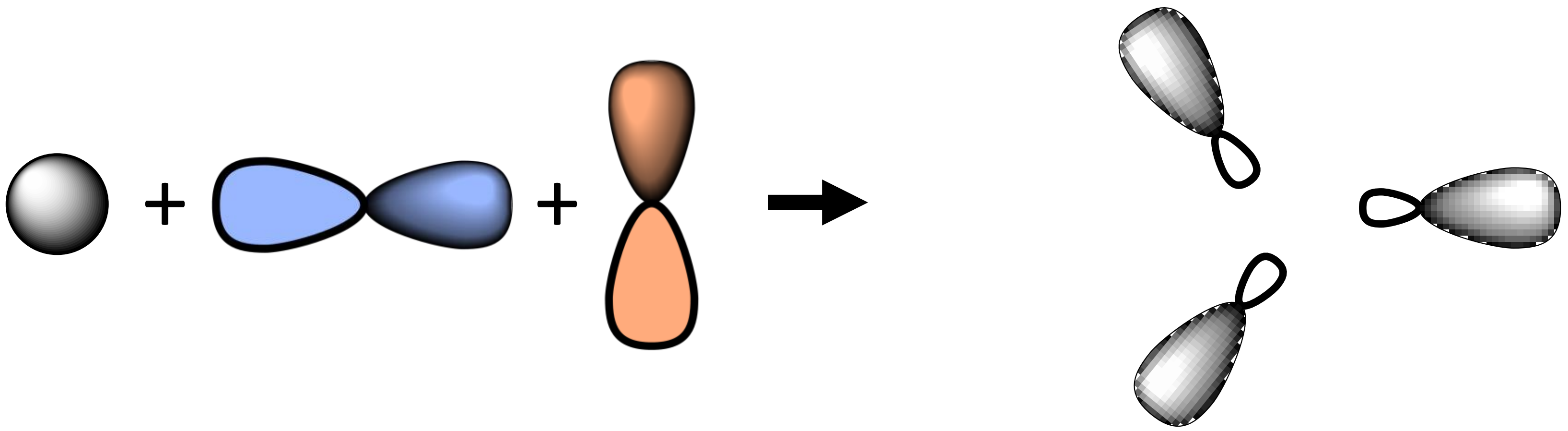
In order to explain the observed geometry of molecules, we can use *hybrid orbital theory*.

In this theory, atomic orbitals are combined to form as many equivalent hybrid orbitals as are needed to form σ bonds and hold lone pairs on the central atom. They are named for the orbitals that were combined to form them:

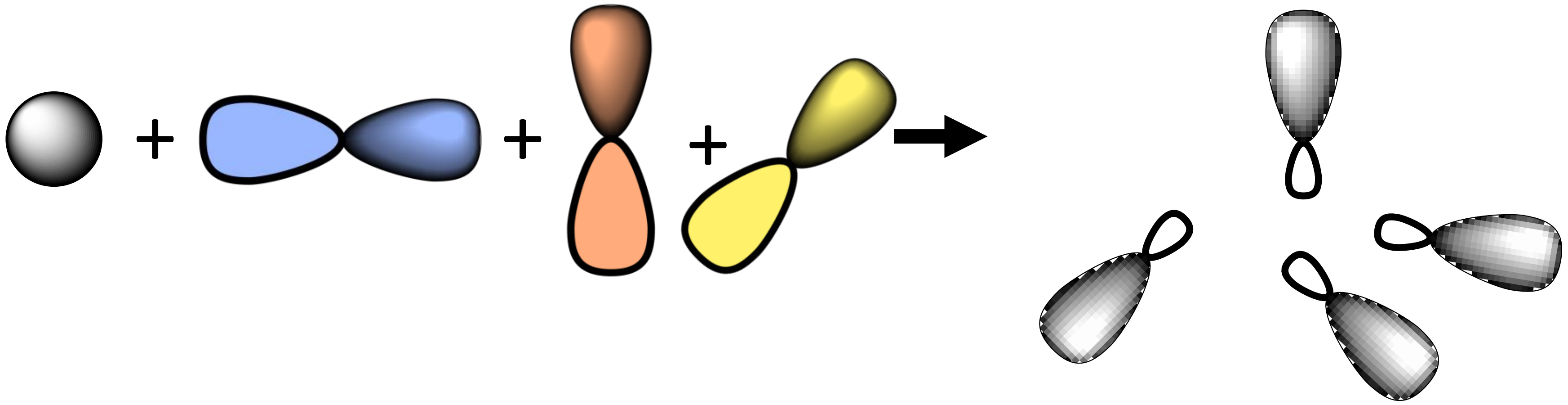
sp hybridization:



sp^2 hybridization:



sp^3 hybridization:



What is the hybridization of the N in NF_3?

a. s (unhybridized)

b. sp

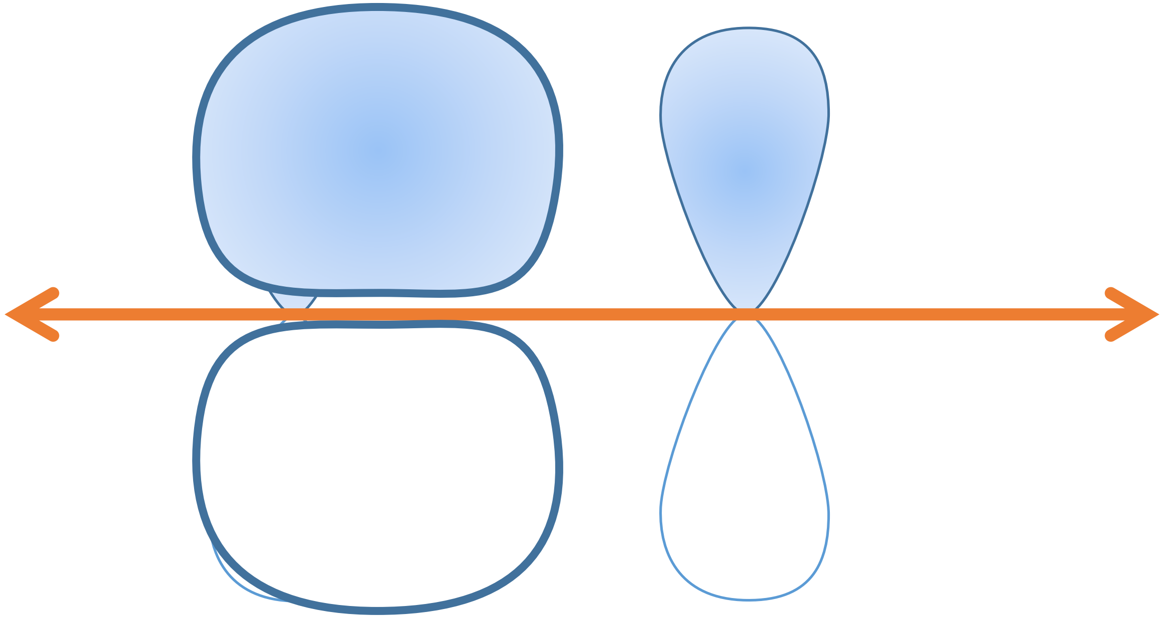
c. sp^2

d. sp^3

What about Double Bonds?

We can't have orbitals overlapping in the same space at the same time!

Double bonds, or π-bonds, "sandwich" a sigma bond, using *p* orbitals:



$\pi_{2p\text{-}2p}$

π bond:

orbital overlap lies *above and below* the internuclear axis

Bonding in ethene:

C_2H_4