The description of a molecule using LE model involves three distinct steps:

1. Draw the Lewis structure(s).
2. Determine the arrangement of electron pairs using VSEPR model
3. Specify the hybrid atomic orbitals needed to accommodate the electron pairs.

An atom in a molecule may adapt a different set of atomic orbitals (hybrid orbitals) from those it has in the free state to achieve minimum energy for the molecule.

Hybridization is a modification of the LE model to account for the observation that atoms often seem to use special atomic orbitals in forming bonds.

sp Hybridization

Two effective pairs around an atom will always require sp hybridization (resulting in linear shape).

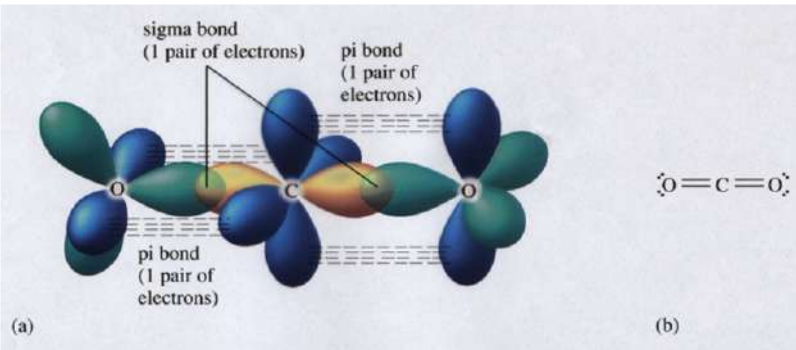
___ ___ ___ 2p ___ ___ 2p unhyb p

E → hybridization ___ ___ sp hybrid

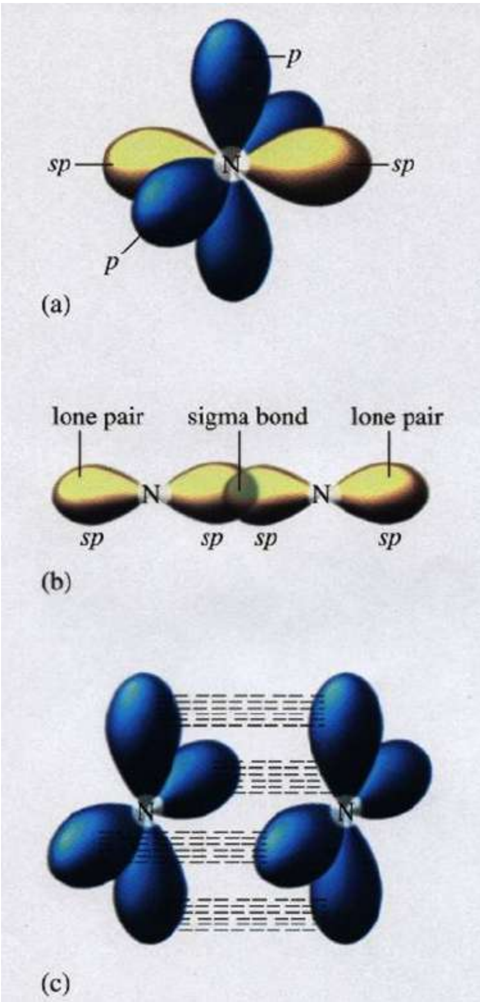
___ 2s

Example: carbon dioxide

— = ≡ :
one e pair



gold = sp
green = sp^2
blue = unhyb p



:N≡N:

Note:

1. sigma (σ) bonds form from overlap of hybrid orbitals
2. bonds formed by the overlap of unhybridized p orbitals (above and below the center plane) are called pi (π) bonds.
3. A single bond is a sigma bond
4. A double bond consists of one σ and one π bond.
5. A triple bond consists of one σ and two π bonds.

σ bonds are formed from orbitals whose lobes point toward each other but π bonds result from parallel orbits.

sp^2 Hybridization

Whenever an atom is surrounded by three effective electron pairs, a set of sp^2 hybrid orbitals is required (which gives a trigonal planar geometry). This leaves

E

___ ___ ___ 2p

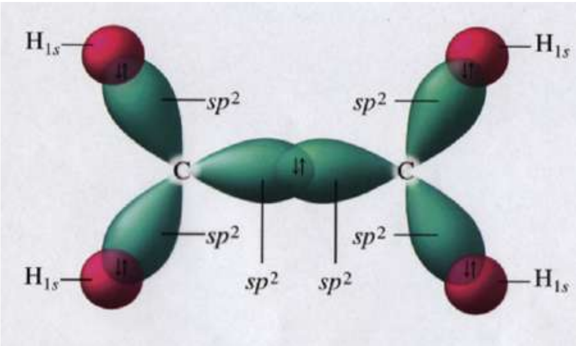
___ 2s

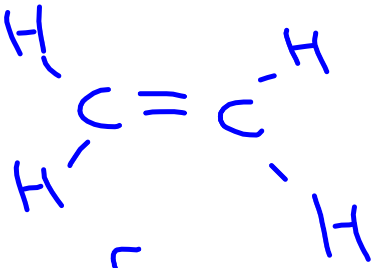
→ hybridization

___ 2p unhyb p

___ ___ ___ sp^2 hybrid

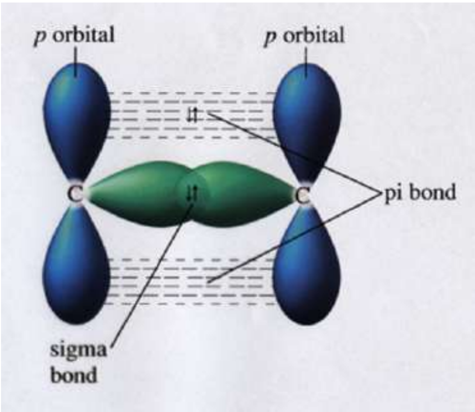
Example: ethylene, C_2H_4



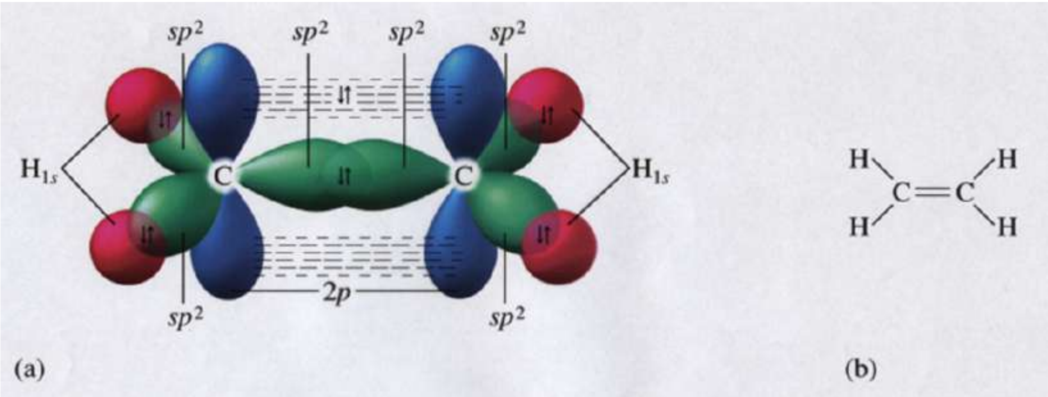


5 σ

1 π

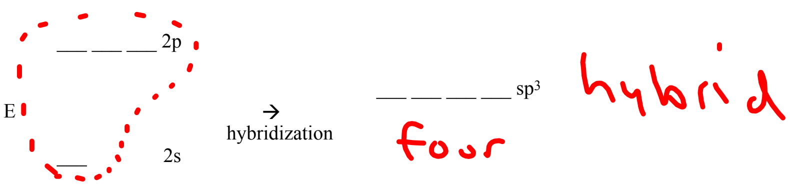


combined:

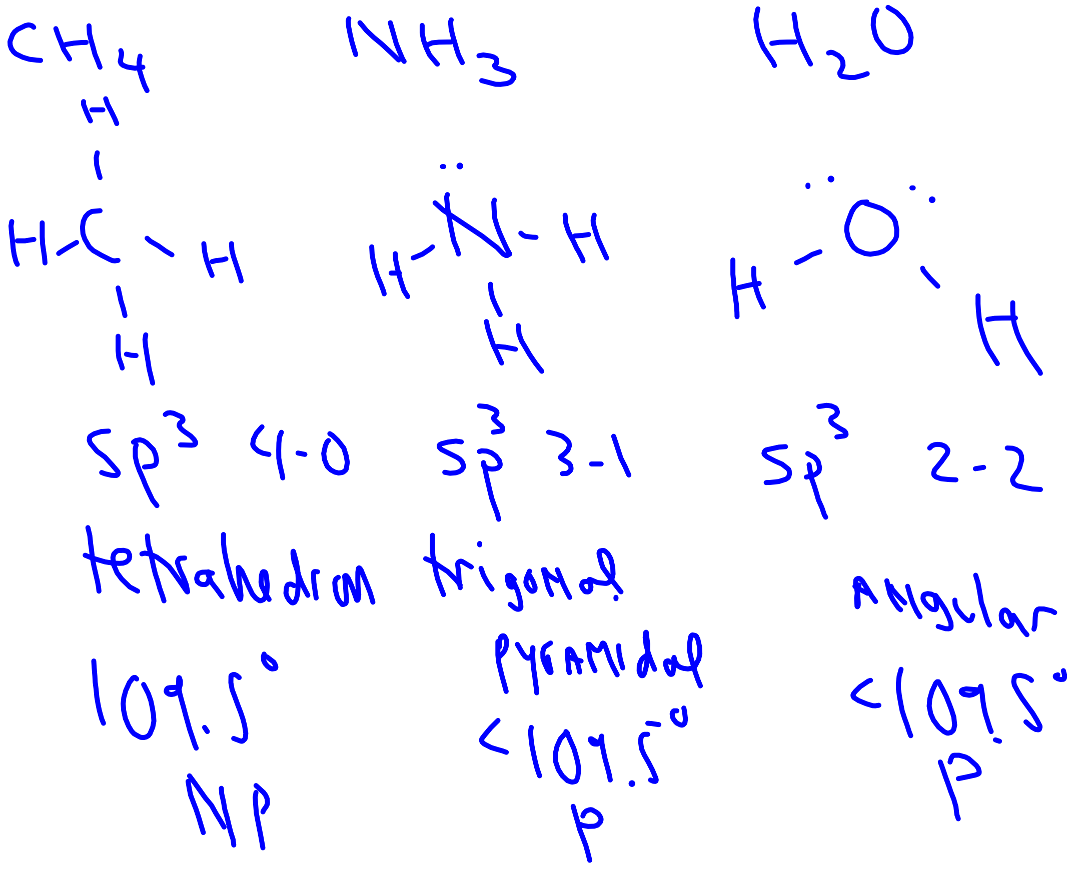


sp^3 Hybridization

Whenever an atom is surrounded by four effective electron pairs, a set of sp^3 hybrid orbitals is required (which gives a tetrahedral geometry). If the four hybrid



Problem: Describe bonding in the methane, ammonia, and water molecules using the LE model.



dsp^3 Hybridization

A set of five effective pairs around a given atom always requires a trigonal bipyramid arrangement of orbitals which in turn requires dsp^3 hybridization of that

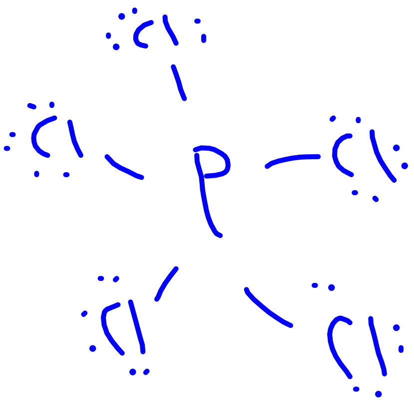
___ ___ ___ ___ ___ 3d   ___ ___ ___ ___ 3d

___ ___ ___ 3p   ___ ___ ___ ___ ___ dsp^3 hybrid

E   → hybridization   five

___ 3s

example: PCl_5



trigonal bipyramid

NP 90°, 120°

d^2sp^3 Hybridization

Six electron pairs around an atom are always arranged octahedrally and require d^2sp^3 hybridization of the atom (octahedron).

___ ___ ___ ___ ___ 3d ___ ___ ___ 3d

___ ___ ___ ___ ___ ___ d^2sp^3 hybrid

E ___ ___ ___ 3p six

→ hybridization

___ 3s

Octahedron

90°

NP

example SF_6

The main idea behind all orbital hybridization schemes is that the hybridization of the orbitals of an atoms depends on the total number of effective electron pairs arc

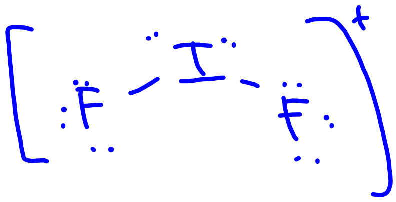
The table below summarizes effective electron pairs around an atom with hybridization. Remember that for purposes of the VSEPR model, double and triple

Effective Electron Pairs Around an Atom	Arrangement *of Orbitals*	Hybridization
2	linear	sp
3	trigonal planar	sp^2
4	tetrahedral	sp^3
5	trigonal bipyramid	dsp^3
6	octahedral	d^2sp^3

Problem: Give the hybridization and predict the geometry of each of the atoms in the following molecules or ions:

a) IF_2^+

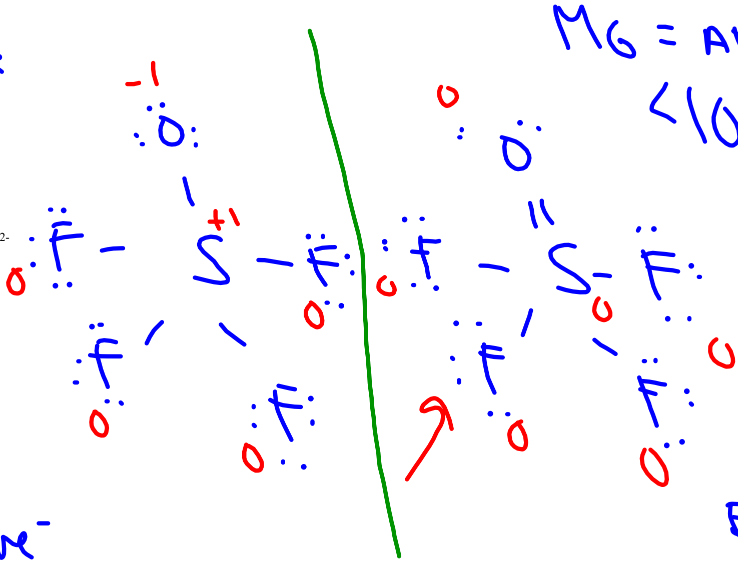
20ve



I is sp^3 2σ
F is sp^3
EPG = tetrahedron
MG = Angular
<109.5° polar

b) $O\underline{S}F_4$

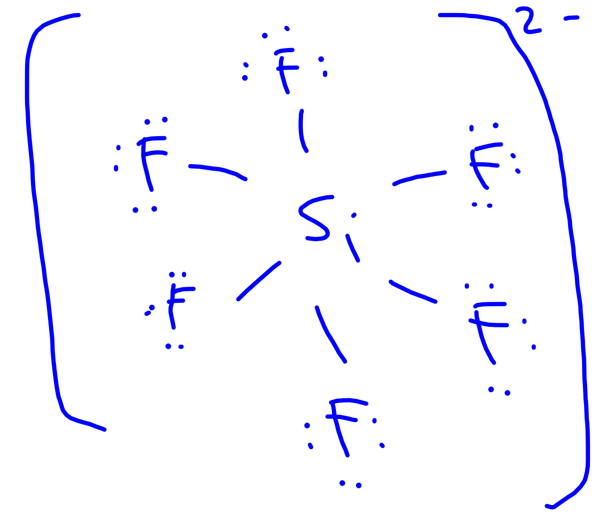
40ve



S = dsp^3
O = sp^2
F = sp^3
EPG = trigonal bipyramid
MG:
120° 90°
polar 5σ 1π

c) SiF_6^{2-}

48ve⁻



Si = d^2sp^3
F = sp^3
EPG = octahedron
MG =
90° NP
6σ