Formal charge (FC):

- A method used to determine the most likely possible Lewis structure
- Based on minimizing the difference in electronegativity.

Steps:

1. Draw a possible Lewis structure.
2. Calculate the FC for each unique atom, where

$$FC = (\#\ \text{valence}\ e^-) - \tfrac{1}{2}(\#\ \text{bonding}\ e^-) - (\#\ \text{non-bonding}\ e^-)$$

3. The Lewis structure with the difference in FC (ΔFC) closest to zero will be preferred.

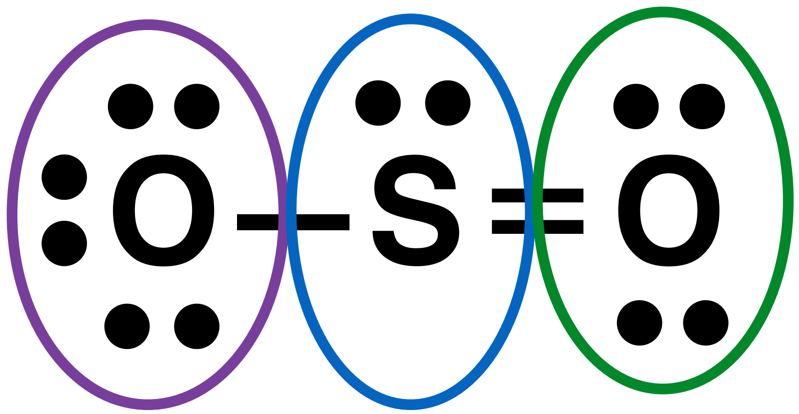
Where,

$$\Delta FC = FC_{max} - FC_{min}$$

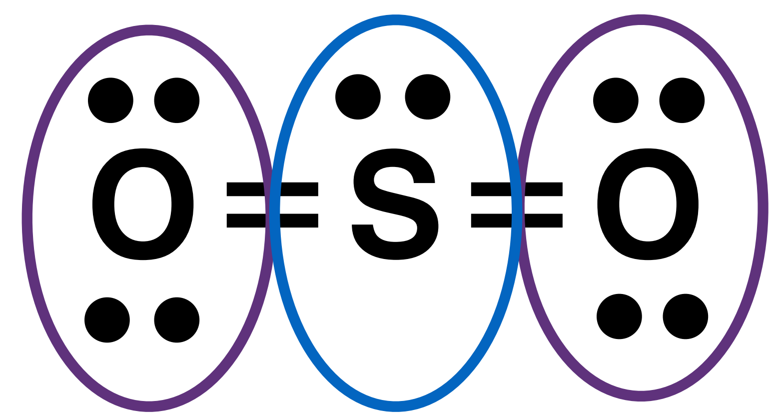
When two Lewis structures have the same ΔFC, choose the one that has the more negative charge on the most electronegative element.

Practice

Use formal charge to determine the more likely Lewis structure for SO_2



or



FC(O–) = 6 – 7 = -1

FC(S) = 6 – 5 = +1

FC(=O) = 6 – 6 = 0

ΔFC = (+1) – (-1) = 2

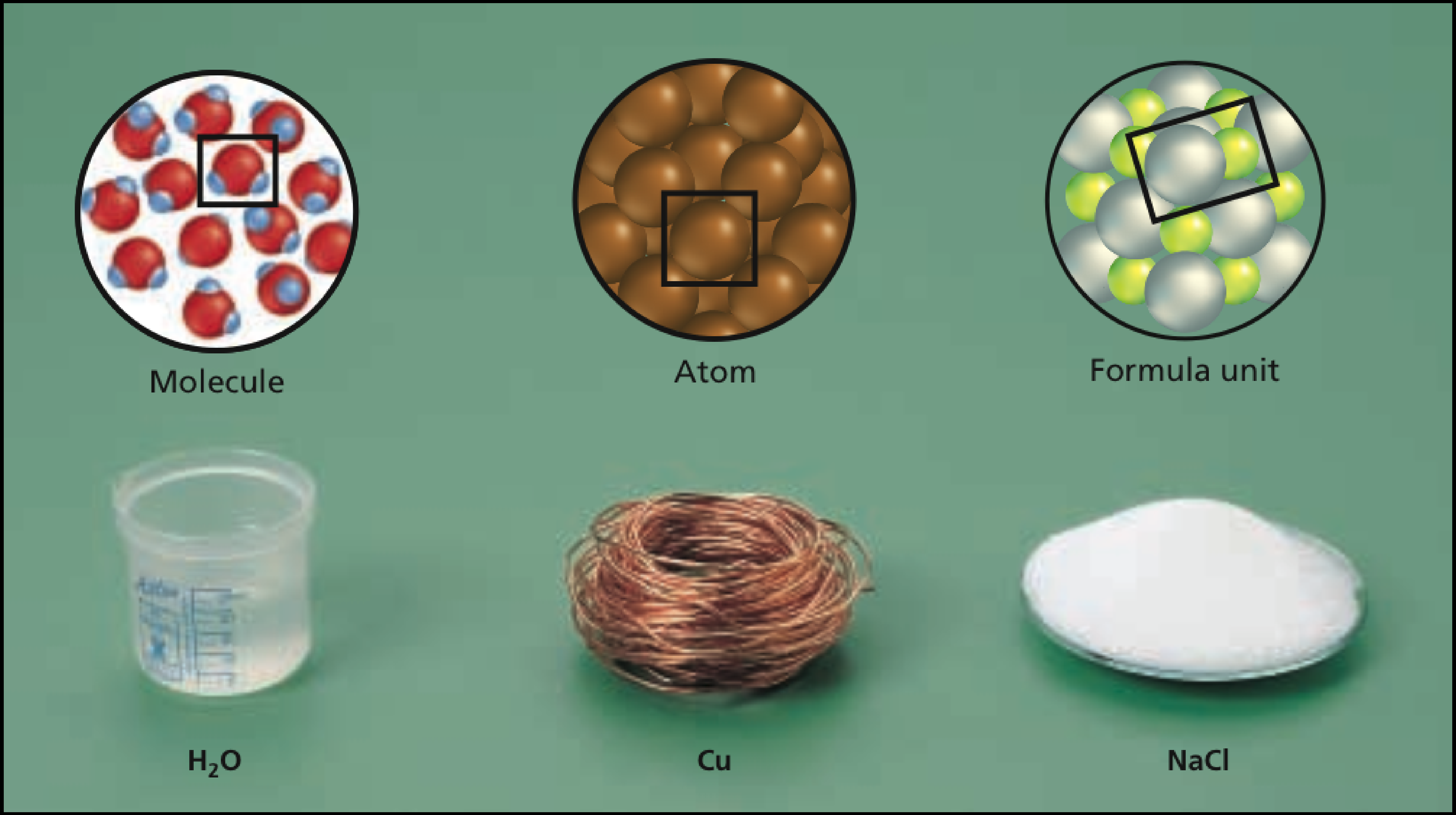
FC(O=) = 6 – 6 = 0

FC(S) = 6 – 6 = 0

more likely structure!

ΔFC = 0 – 0 = 0

Pure Substances

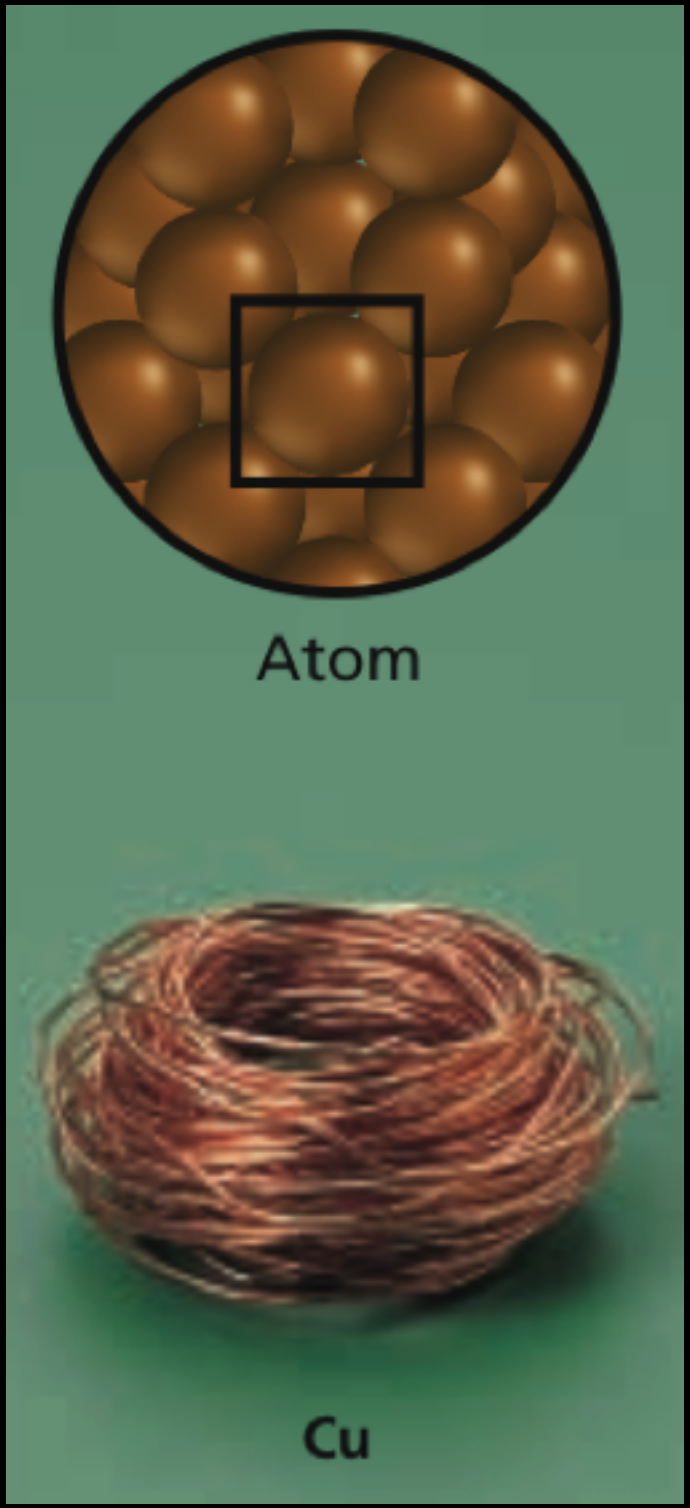


covalent compounds

elements

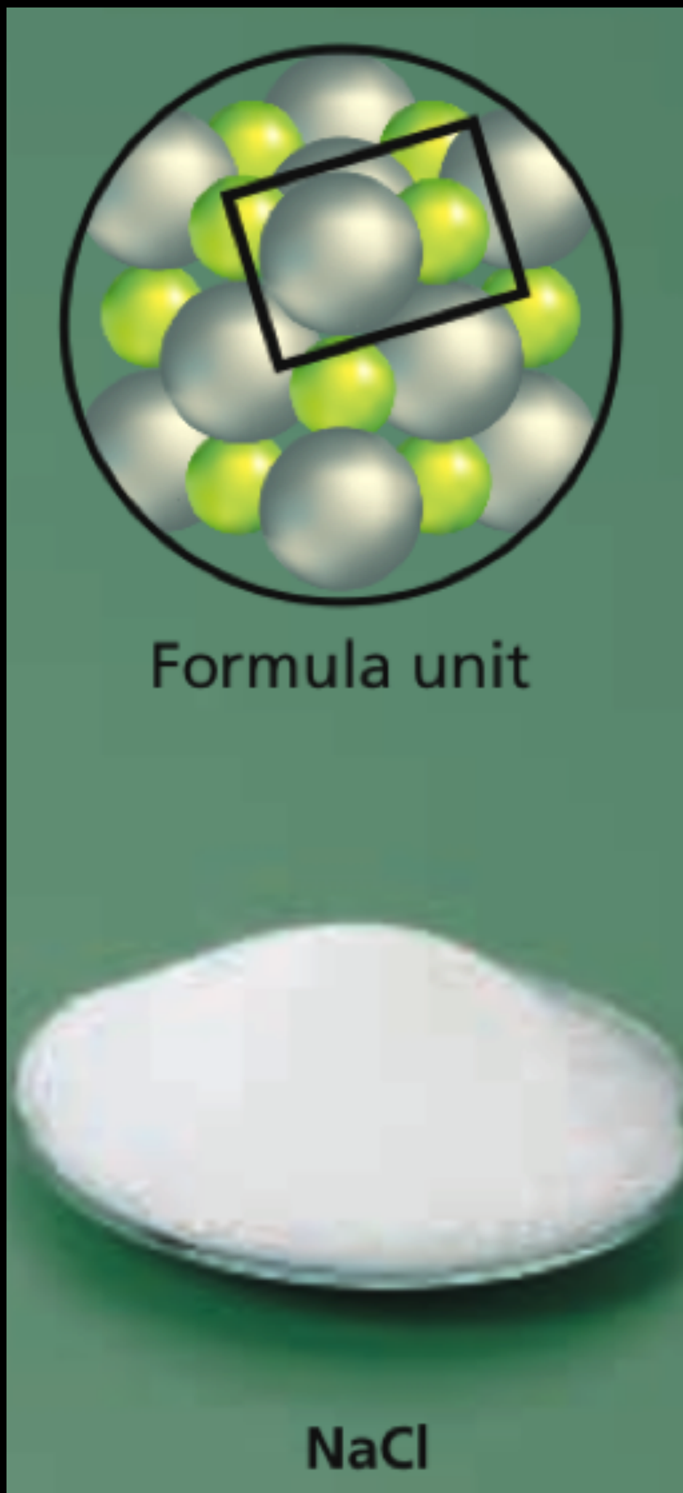
ionic compounds

Pure Substances



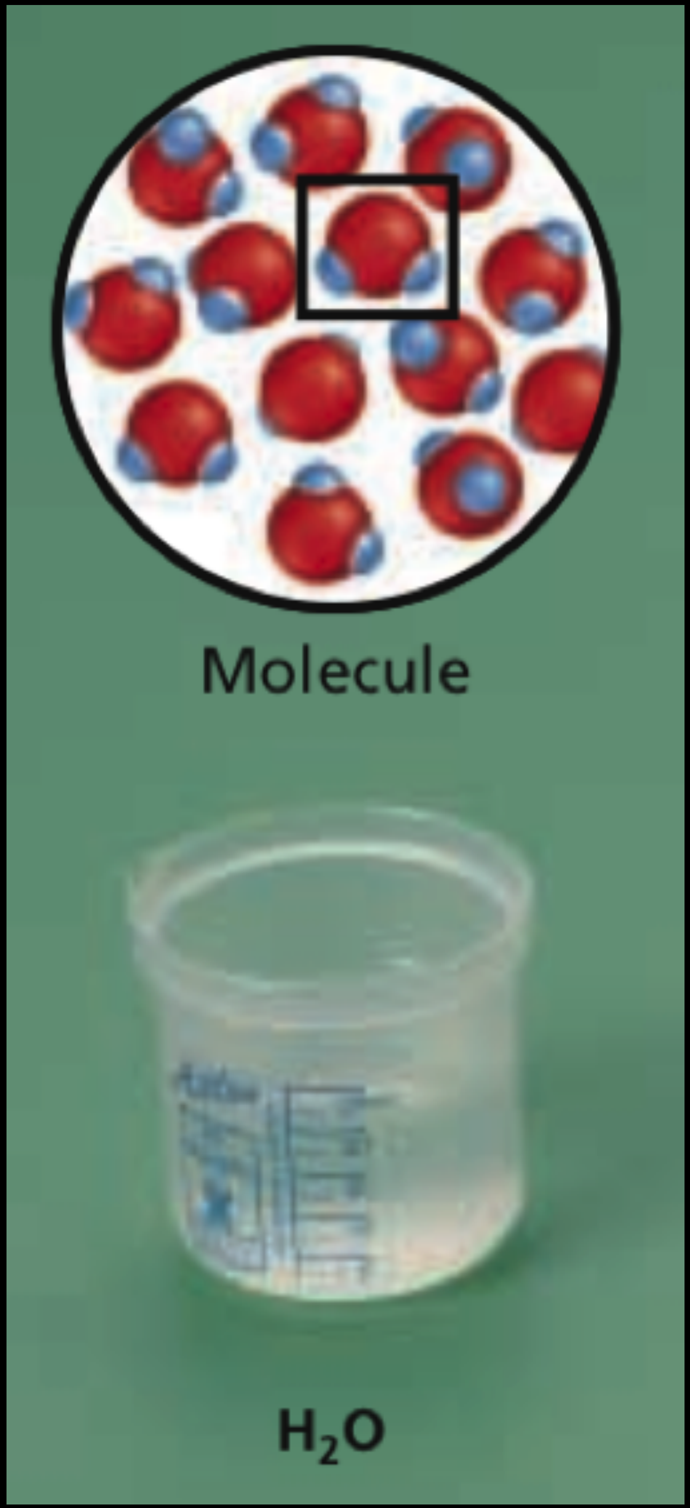
1. Elements contain only one type of atom.

Its chemical formula represents one "atom."



2. Ionic compounds contain metal cations and nonmetal anions.

Its chemical formula represents a "formula unit," the smallest ratio of atoms in its crystal lattice.



3. Covalent (molecular) compounds contain only nonmetals covalently bonded.

Its chemical formula represents one "molecule."

Molecular Structures

Bond length and strength

	Bond length	Bond strength
single bonds	longest	weakest
double bonds	intermediate	intermediate
triple bonds	shortest	strongest

Resonance Structures:

A molecule or polyatomic ion that cannot be represented by a single Lewis structure.

(All will contain a double bond that can be placed on more than one atom)

Lewis Structures for Ozone

Bond energy:

	Bond energy (kJ/mol)
H—F	570
C—F	552
O—O	498
H—H	436
H—Cl	432
C—Cl	397
H—Br	366
H—I	299
C—Br	280
Cl—Cl	243
C—I	209
Br—Br	193
F—F	159
I—I	151

Bond energy:

the energy required to break a chemical bond and form neutral isolated atoms. (reported in kJ/mol)

See page 172

FIGURE 2.5

BOND LENGTHS AND BOND ENERGIES FOR SELECTED COVALENT BONDS

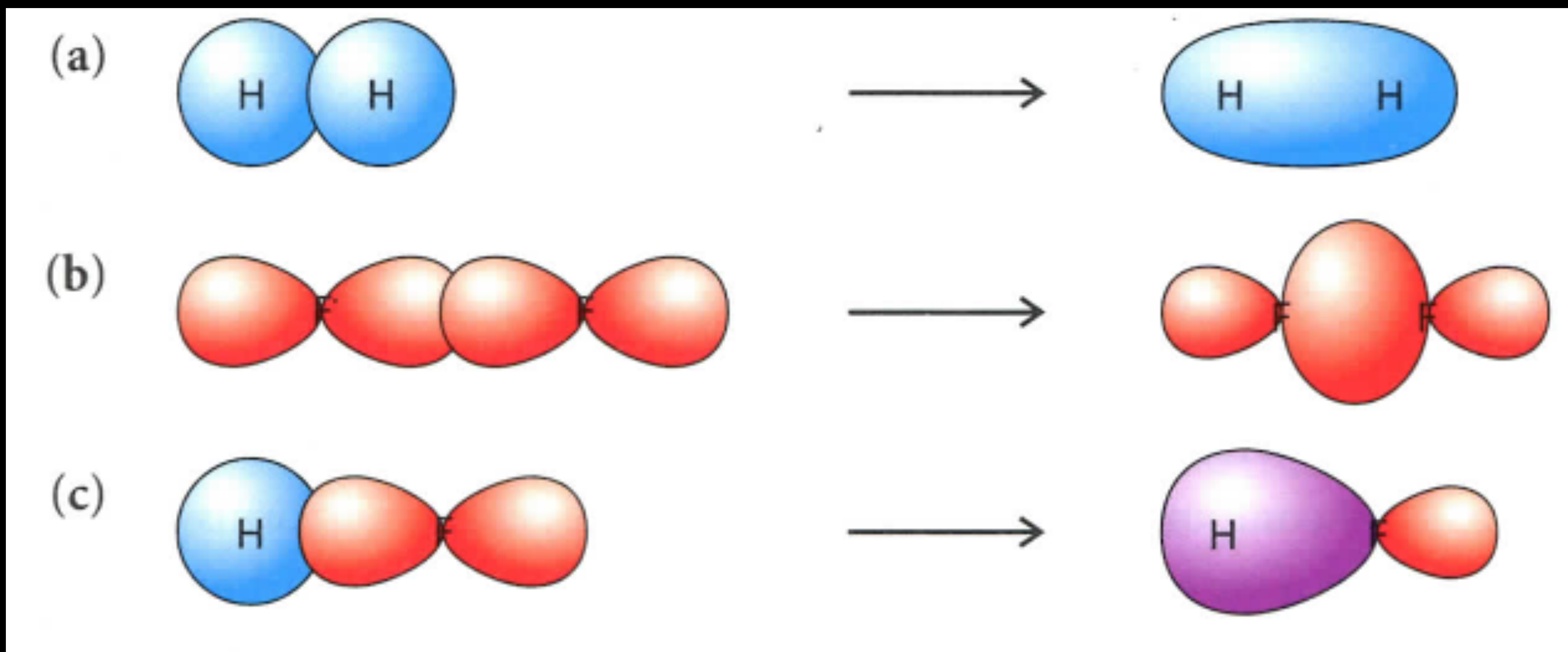
Bond	Average bond length (pm)	Average bond energy (kJ/mol)	Bond	Average bond length (pm)	Average bond energy (kJ/mol)
H—H	75	436	C—C	154	346
F—F	142	159	C—N	147	305
Cl—Cl	199	243	C—O	143	358
Br—Br	229	193	C—H	109	418
I—I	266	151	C—Cl	177	327
H—F	92	569	C—Br	194	285
H—Cl	127	432	N—N	145	163
H—Br	141	366	N—H	101	386
H—I	161	299	O—H	96	459

Note: The greater the bond energy, the shorter the bond length.

Single, double, and triple bonding:

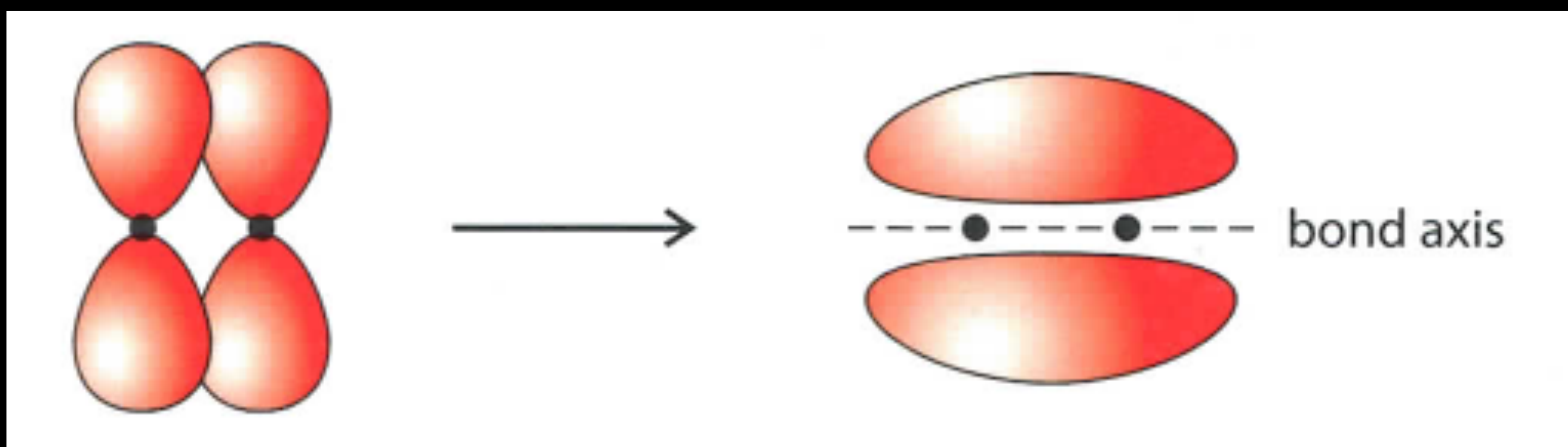
pi and sigma bonds

sigma (σ) bonds resulting from the axial overlap of orbitals:



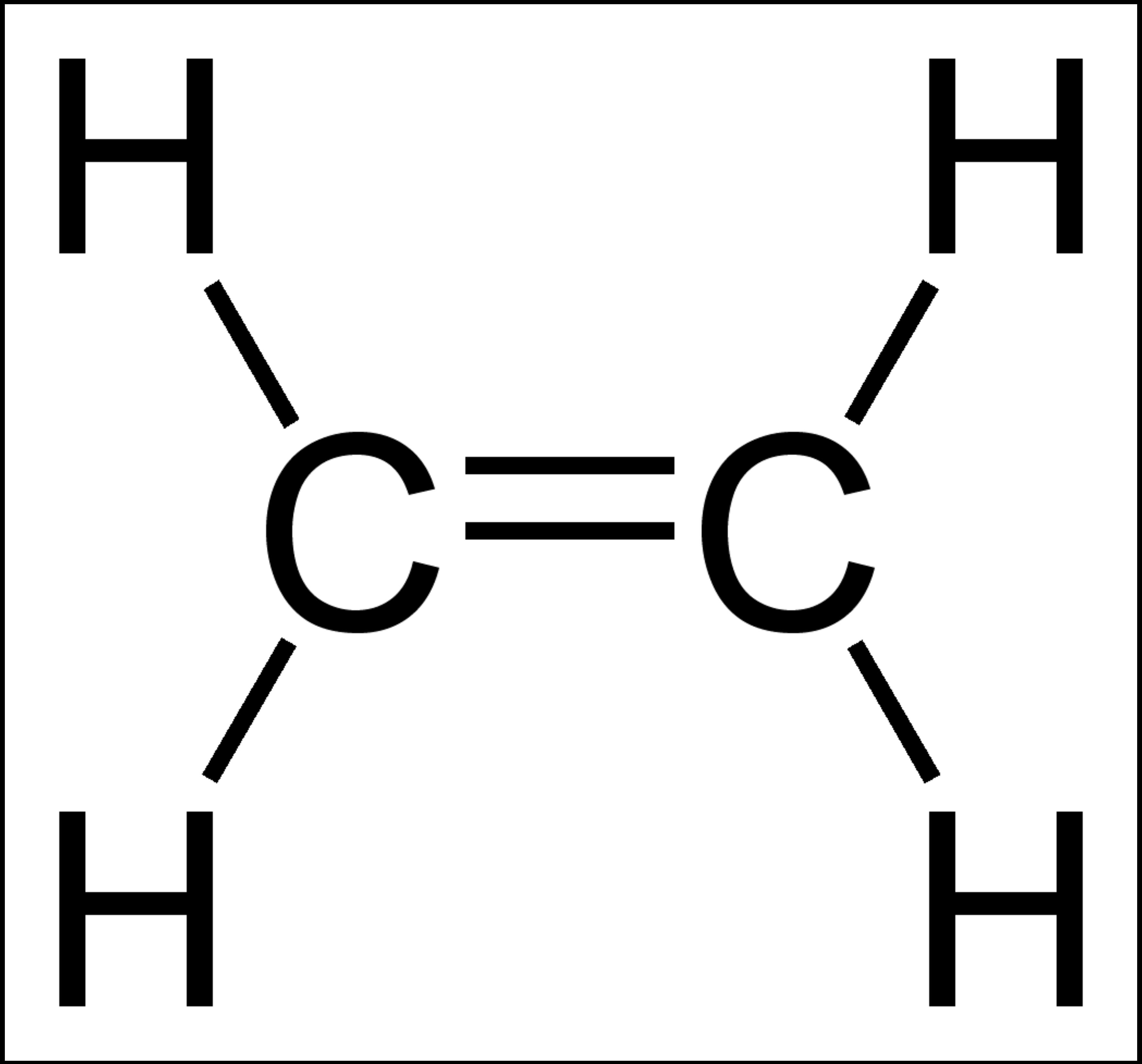
An end-to-end overlapping of s, p, or hybrid orbitals.

pi (π) bonds resulting from the sideways overlap of parallel p orbitals:

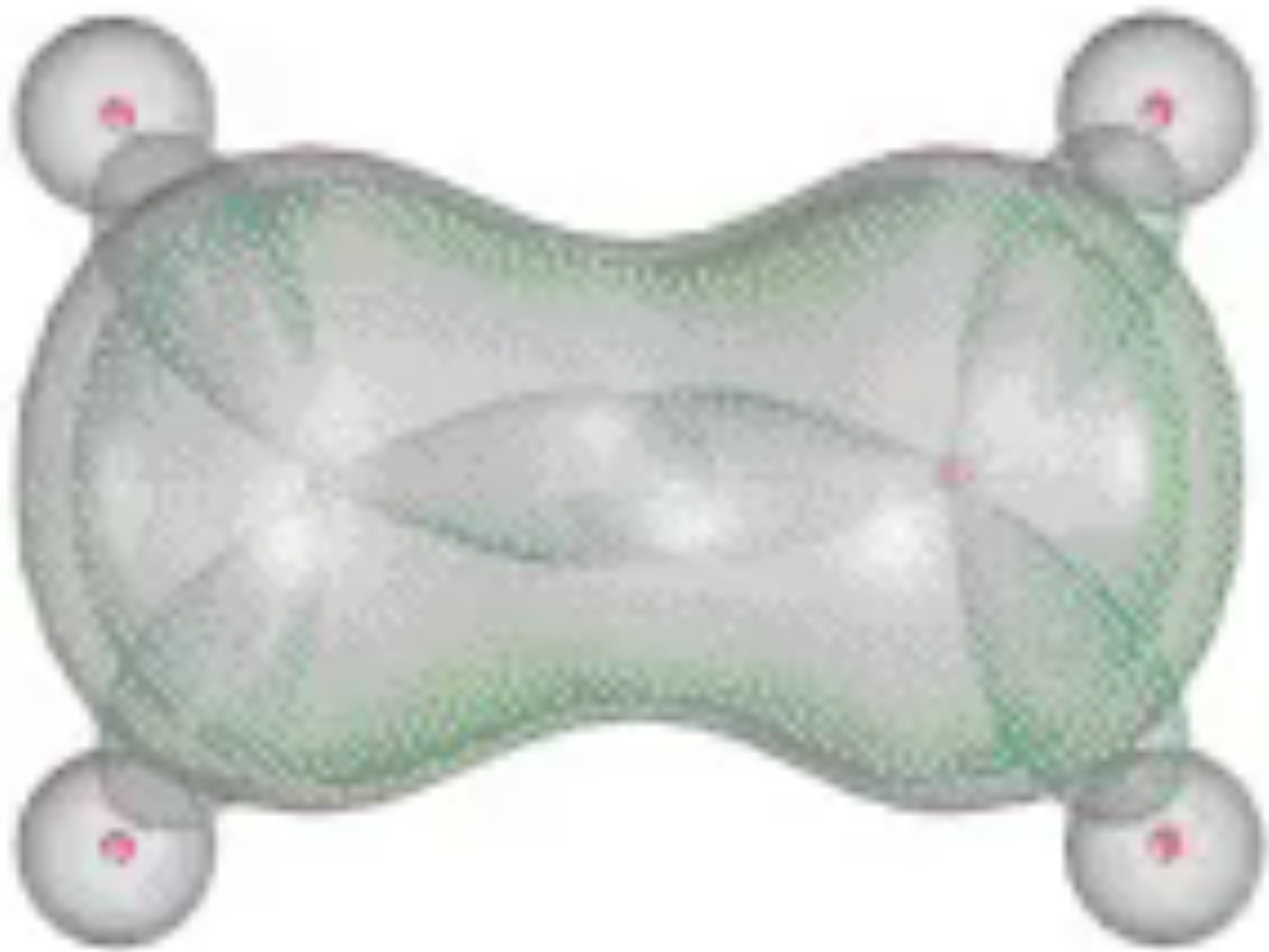


An overlapping of p orbitals above and below a sigma bond.

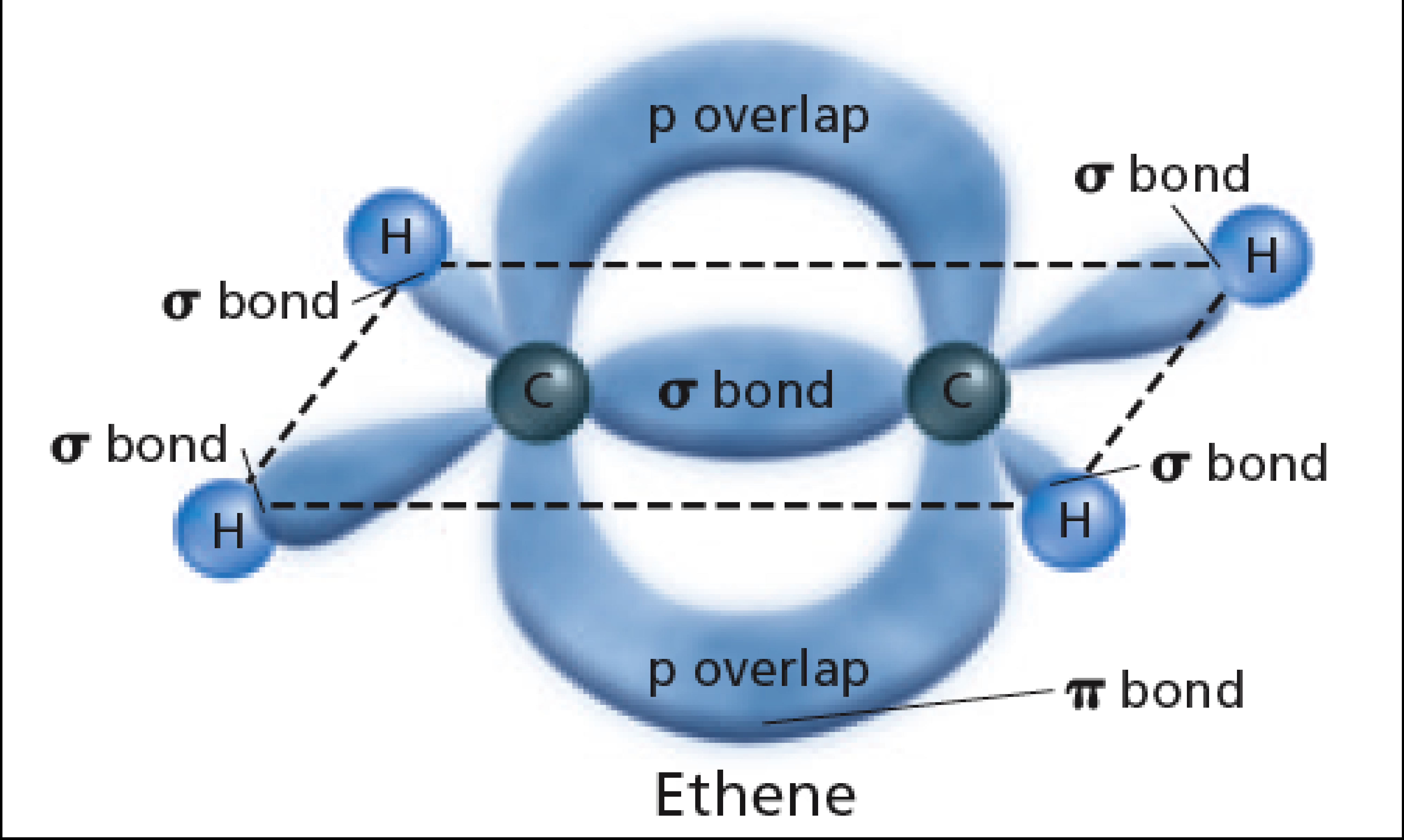
Example: C_2H_4



Example: C_2H_4



Example: C_2H_4



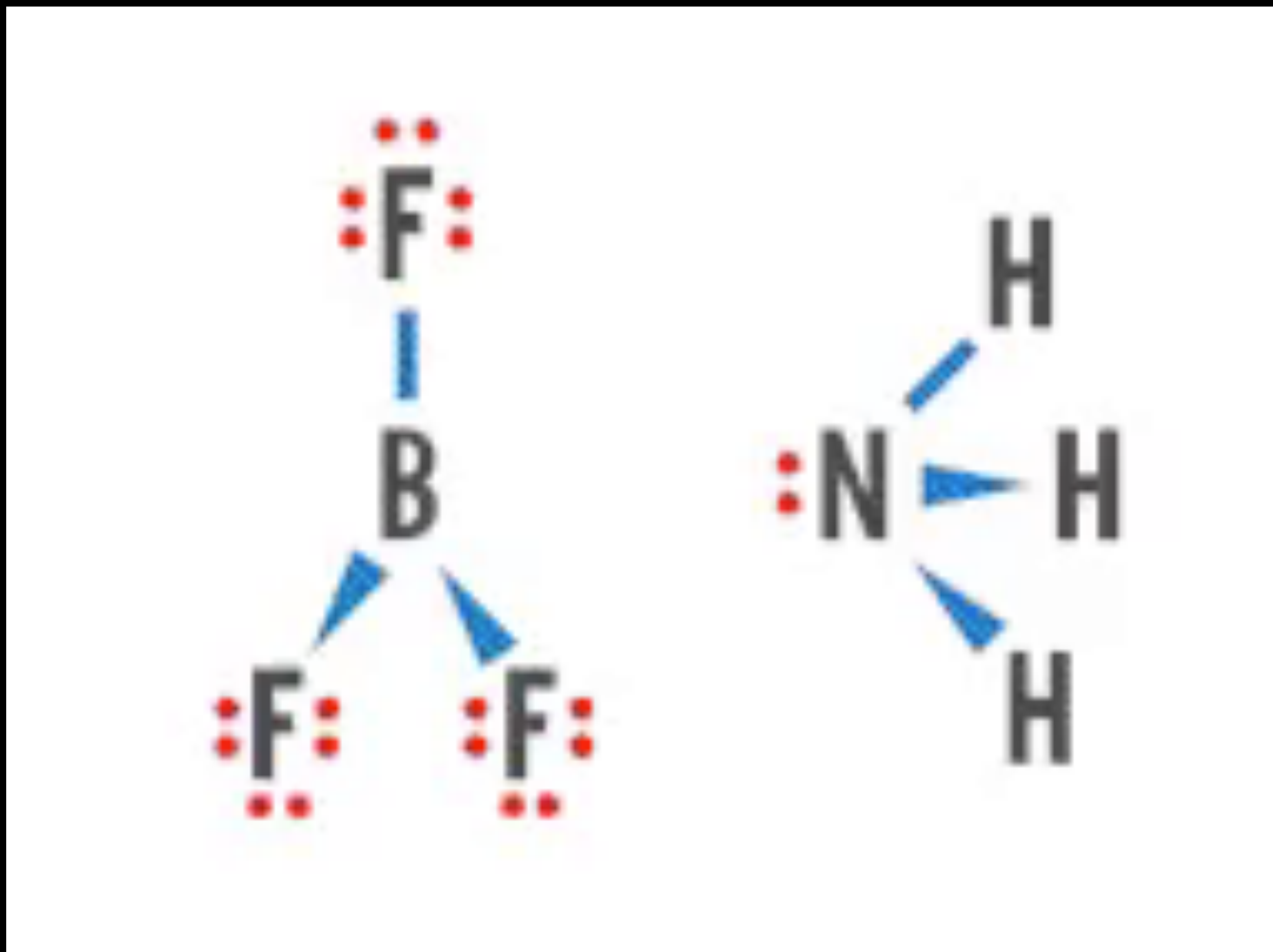
Summary

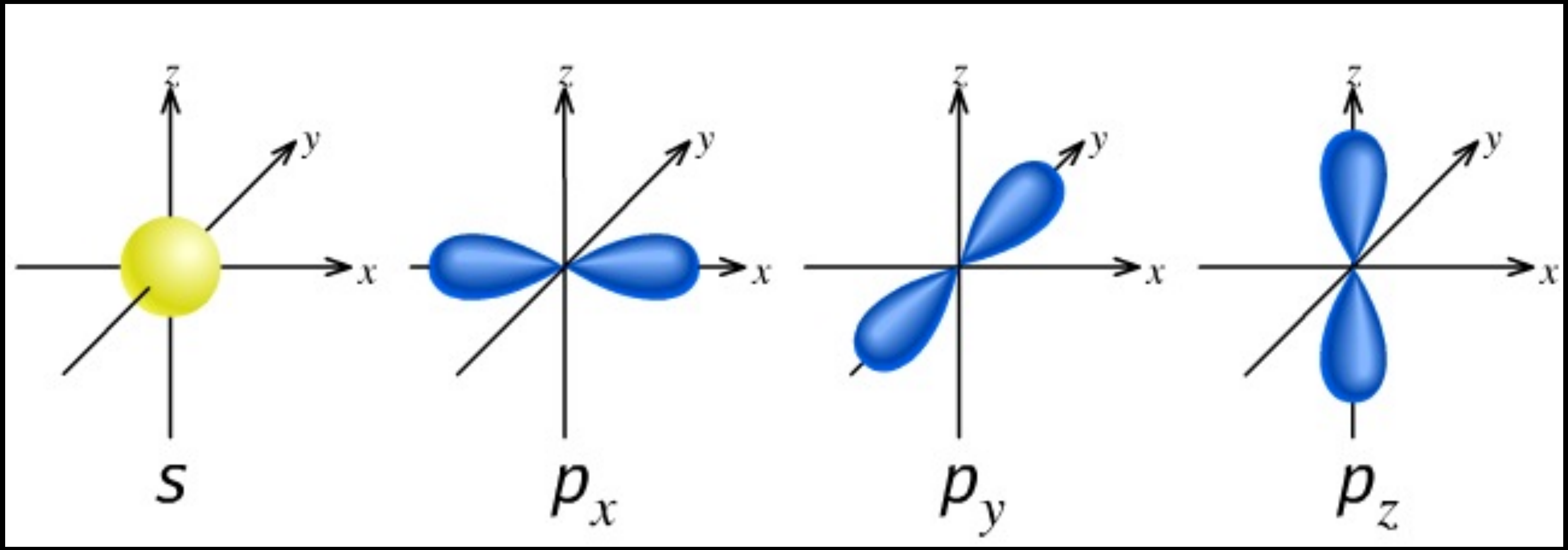
single bonds: one σ bond

double bonds: one σ and one π bond

triple bonds: one σ and two π bonds

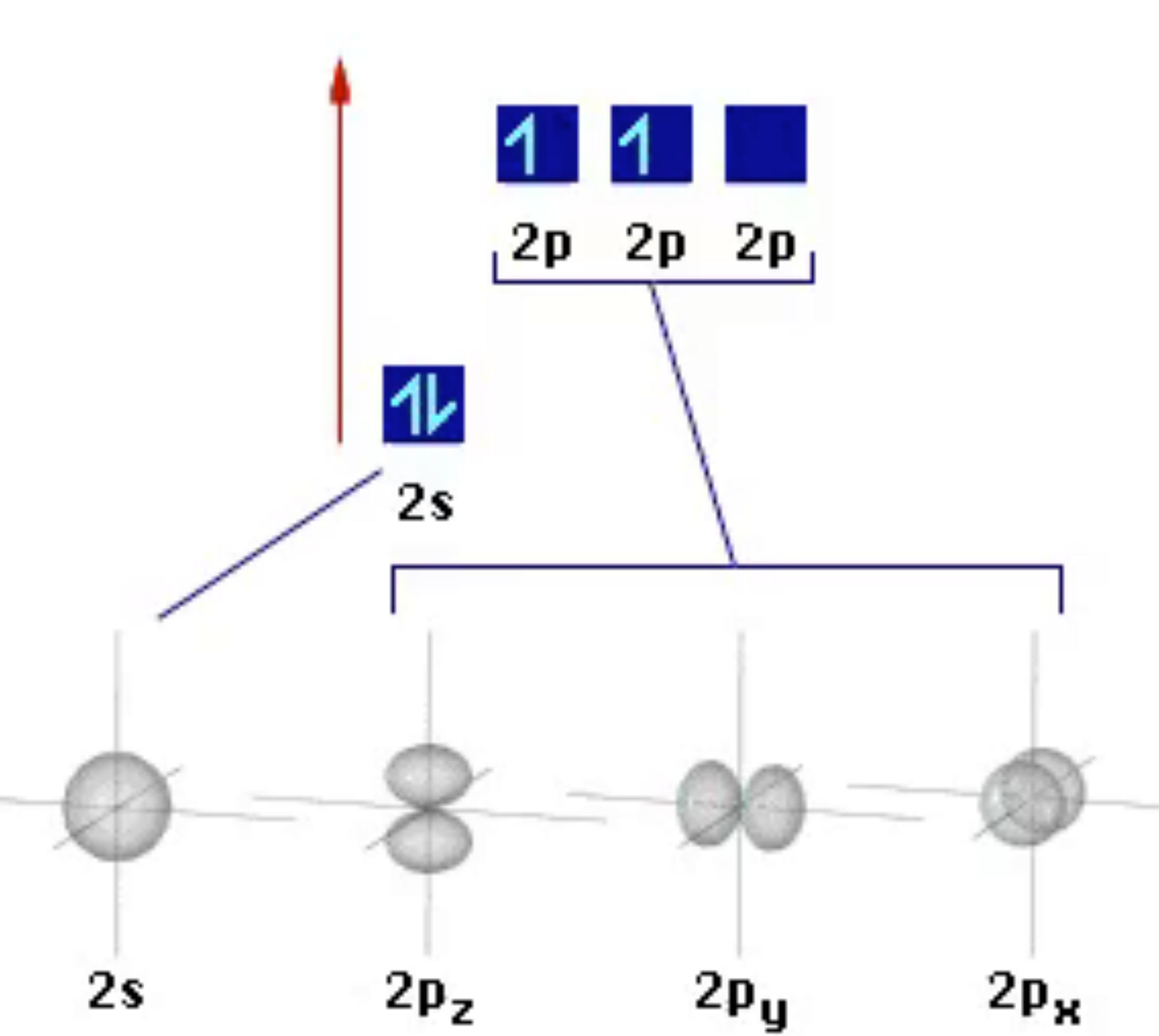
Dative (coordinate) covalent bond: When one atom supplies both electrons in a covalent bond.





Hybridization:

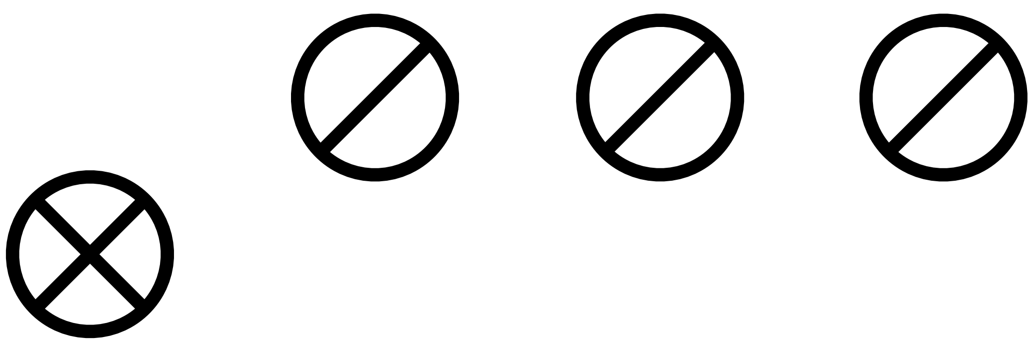
- The mixing of s and p orbitals to form new “hybrid” orbitals.
- Each hybrid orbital is identical and capable for forming a covalent bond



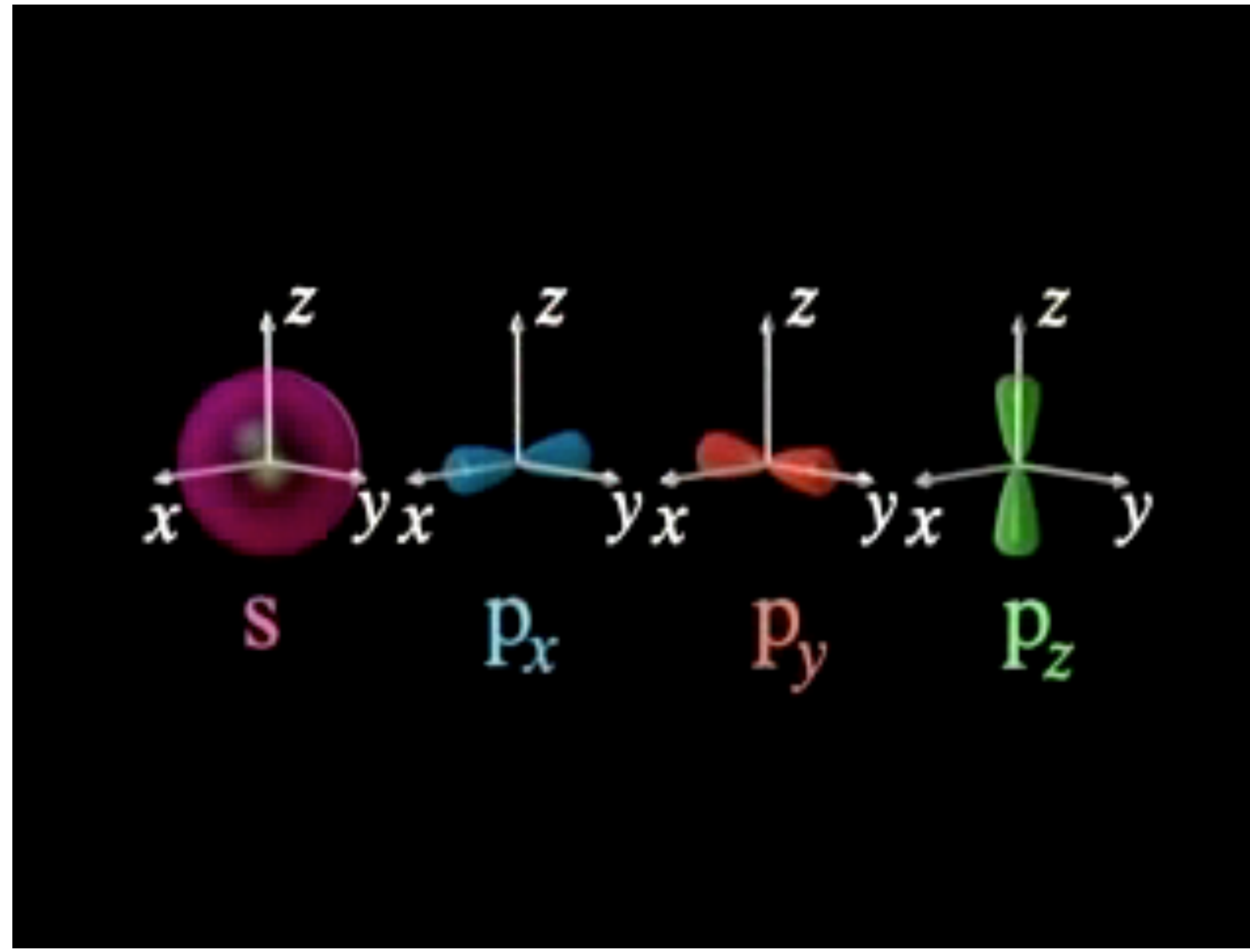
2p
2p
2p
2s
2s
$2p_z$
$2p_y$
$2p_x$

sp^3 Hybridization
Example: CH_4

Four identical bonds in CH_4



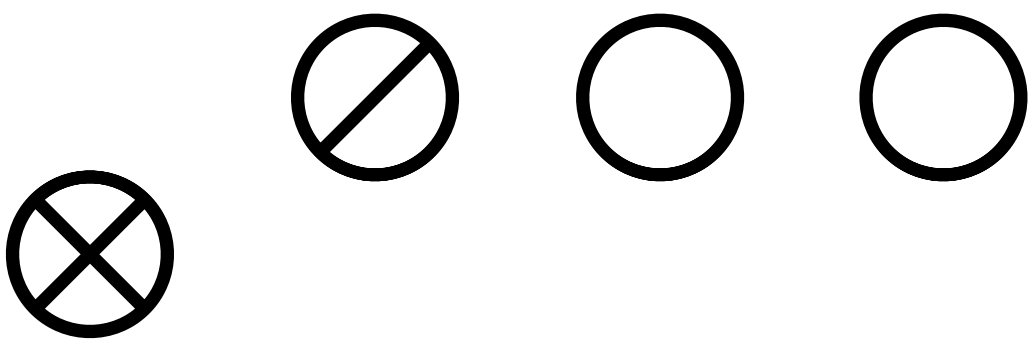
2s **$sp^3$2p**



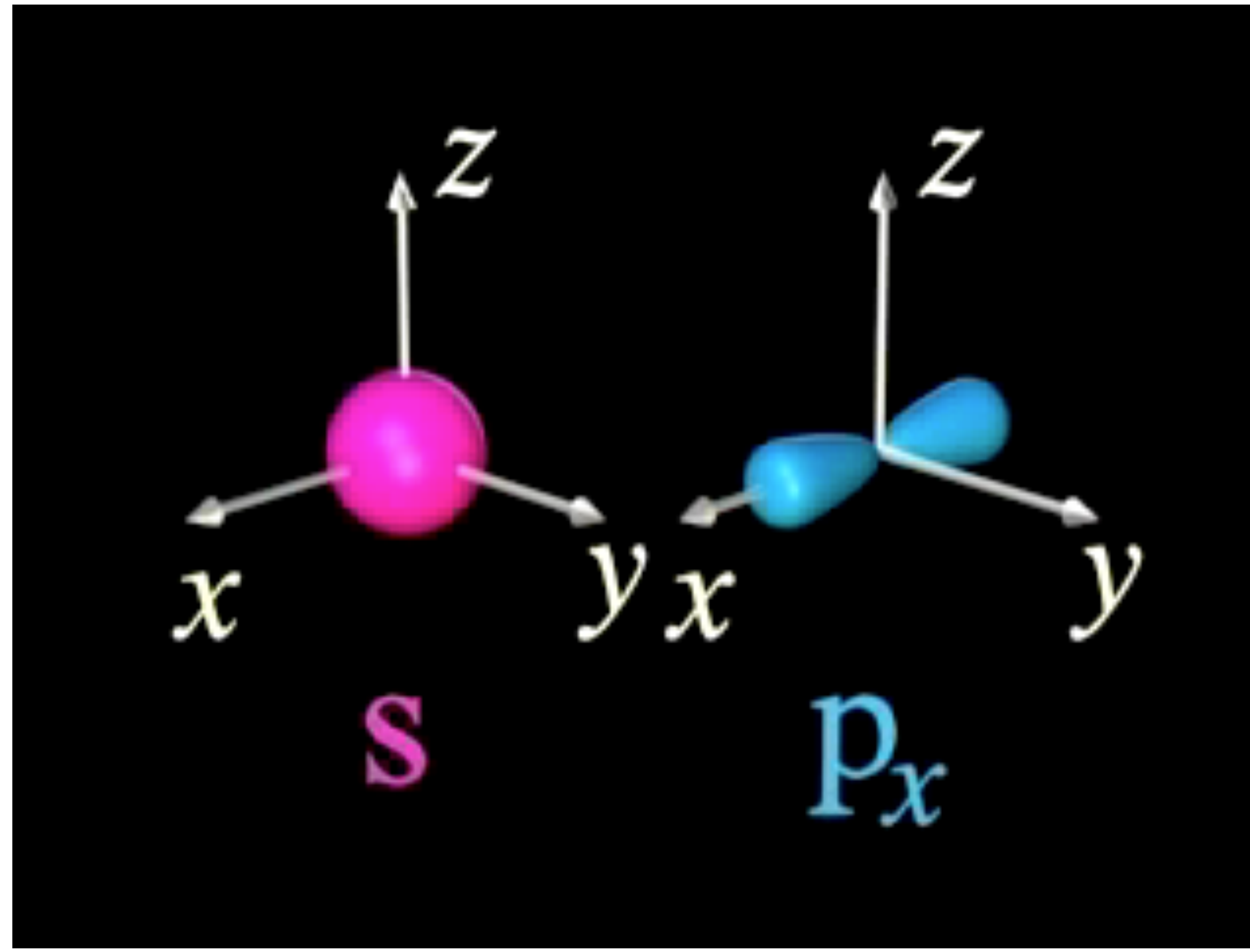
One **s orbital and *three* p orbitals become**
four **identical sp^3 orbitals**

sp Hybridization
Example: BeH_2

Two identical bonds in BeH_2



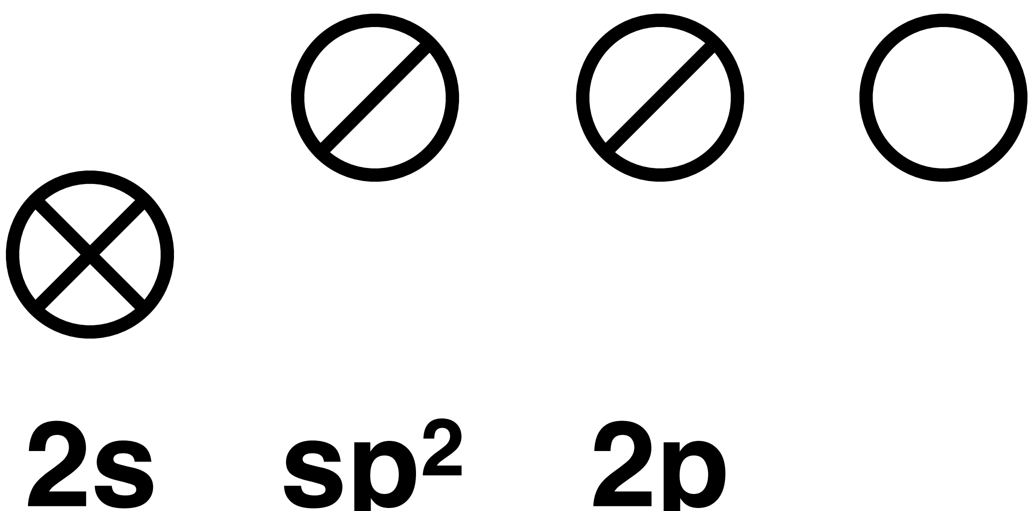
2s sp **2p**

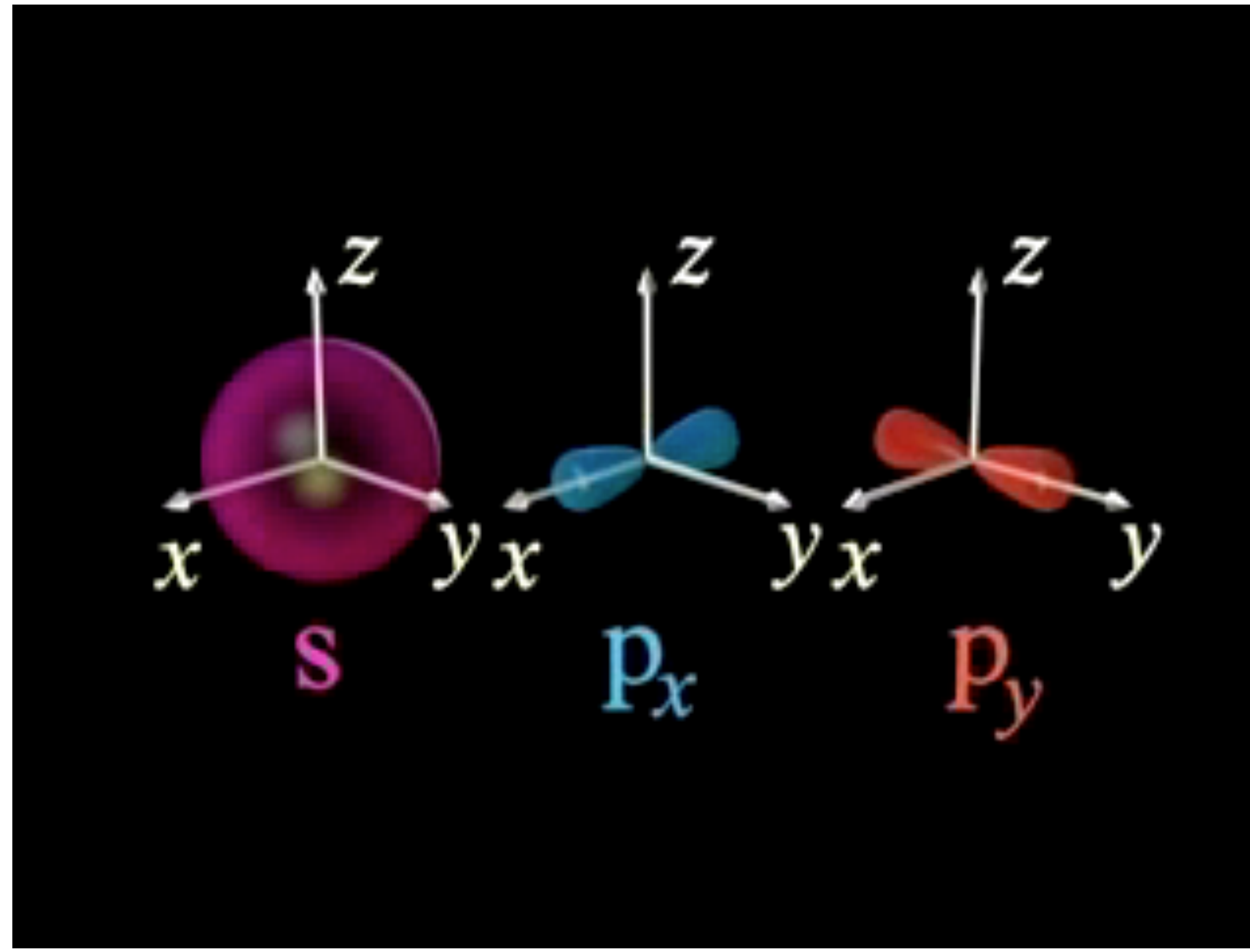


***One* s orbital and *one* p orbital become *two* identical sp orbitals**

sp^2 Hybridization
Example: BCl_3

Three identical bonds in BCl_3





One **s orbital and** ***two*** **p orbitals become** ***three*** **identical sp^2 orbitals**