Appropriate Problems from McMurry Chap 1

Section 1.3 Problems 1-1 and 1-3

Section 1.4 Problems 1-4 through 1-7, 1-24 through 1-28 1-33

Section 1.5 - 1.10 Problems 1-8, 1-9, 1-10, 1-11, 1-12, 1-13, 1-14, 1-34 – 1-40, 1-48, 1-49, 1-50 (part a is asking how are they similar electronically), 1-56

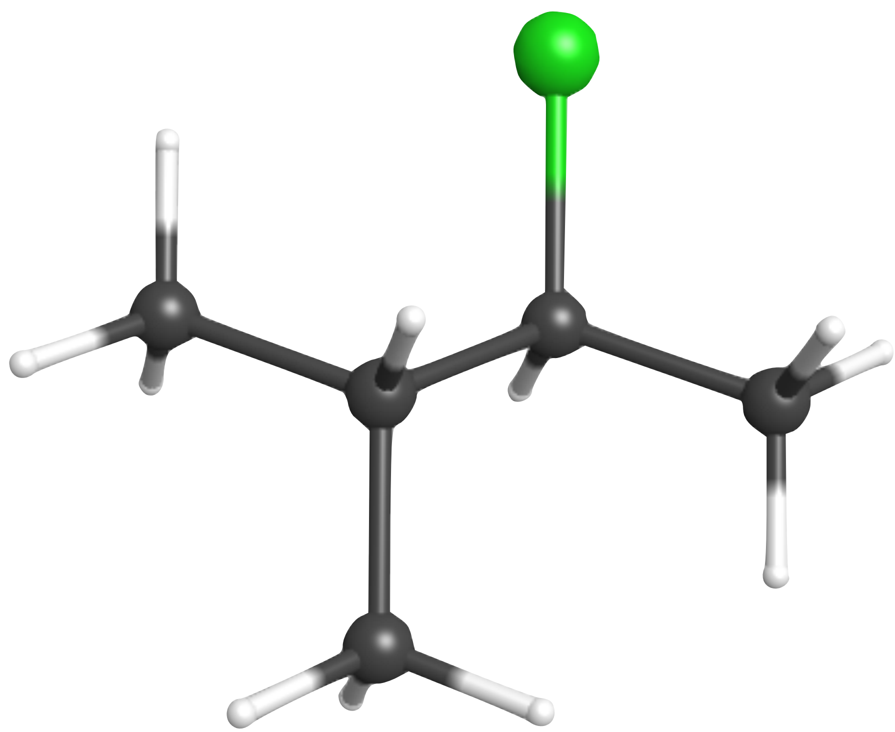
Section 1.12 Problems 1-15 through 1-21, 1-41 through 1-44, 1-52, 1-53, 1-54, 1-55

Challenging Problems 1-45, 1-46, 1-47, 1-51

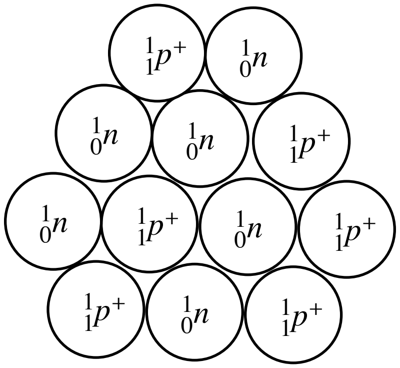
Atoms, Elements, Molecules, and Substituents or Groups

A diversion into the language of chemistry…

“In chemistry, an element is a pure substance consisting only of atoms that all have the same numbers of protons in their atomic nuclei.”[1]

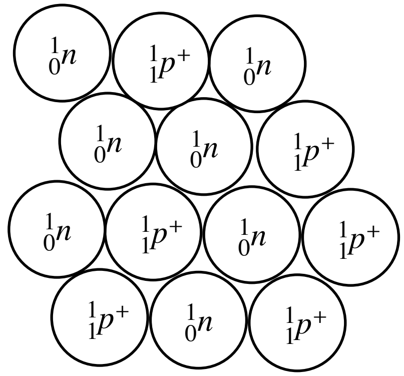


[1] https://en.wikipedia.org/wiki/Chemical_element accessed September 3, 2021



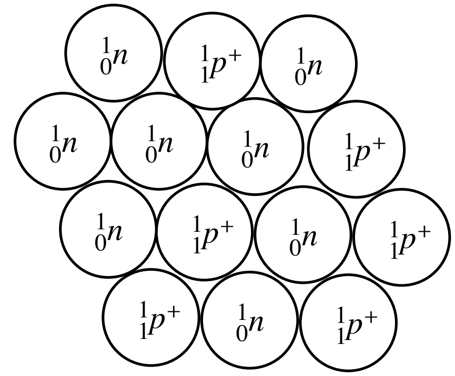
6 protons
6 neutrons

^{12}C



6 protons
7 neutrons

^{13}C

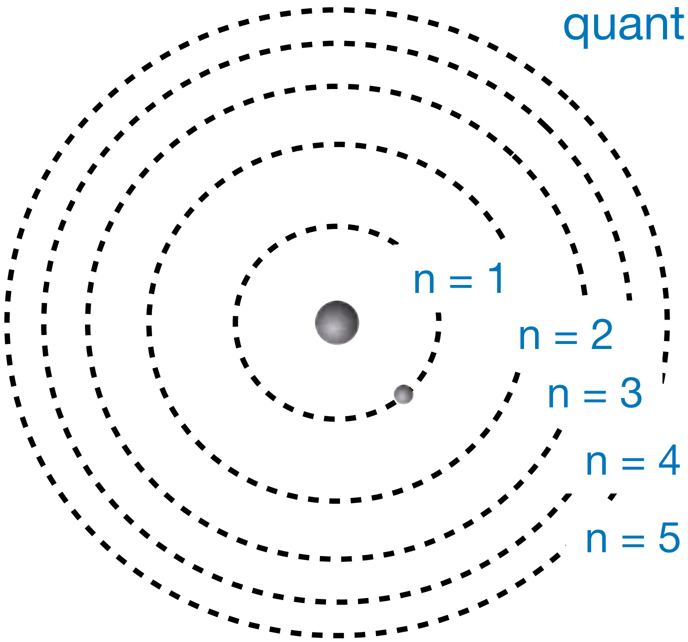


6 protons
8 neutrons

^{14}C

Remember the structure of an atom

Line spectra produced by excited atoms revealed that electrons can only exist in specific energy levels and any model that attempts to describe the atom must have quantized energy levels.



Bohr successfully modeled the Hydrogen atom like a planetary system using particle physics; e.g.,

e^- orbited the atom in defined energy levels

e^- was held in its orbit by electrostatic attraction

E = KE + PE which is $E = 1/2\ mv^2 + Ze^2/r$

The model only worked for atoms with one electron.

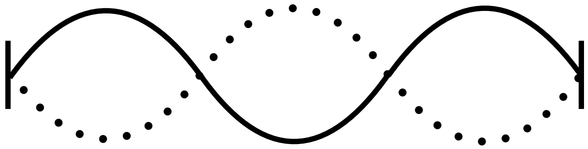
Also it is physically impossible for electrons to orbit a nucleus like the Moon orbits the Earth…. The electrons would radiate energy and crash into the nucleus.

Another branch of Physics also researched systems that had quantized energy levels…

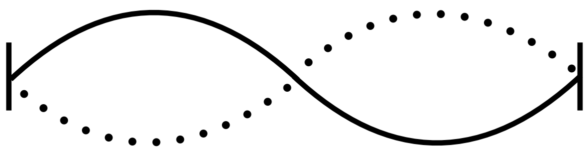
Wave Mechanics

And Where Are the Electrons Again?

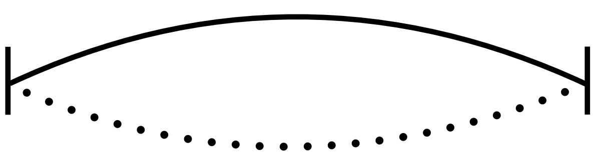
n = 3



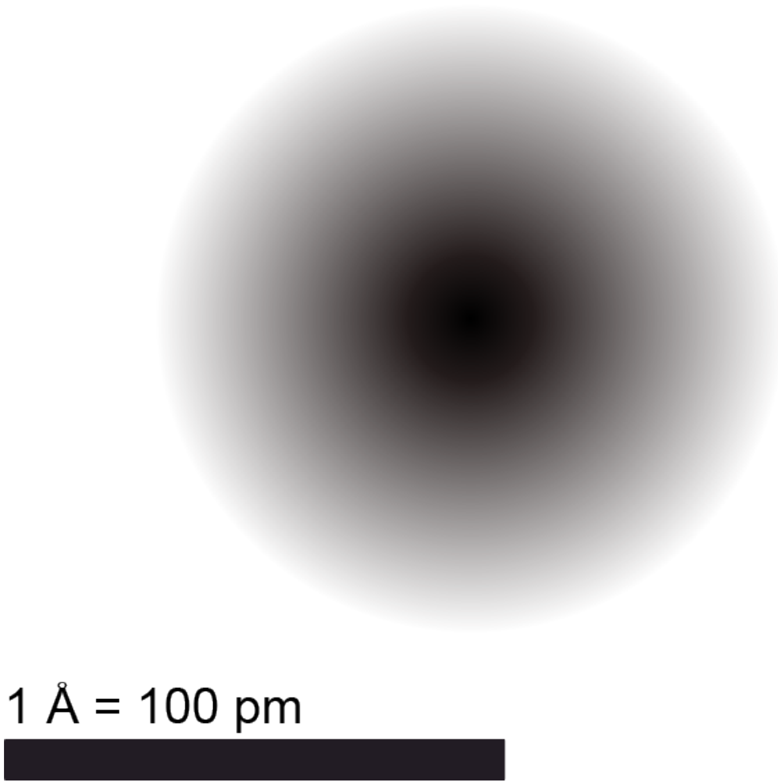
n = 2



n = 1



Wave/Quantum Mechanical Model



Bohr had 1 quantum number.

the electron is in the n = 1 or 2 or 3 or 4… shell

Quantum Mechanics requires four quantum numbers to describe an electron: n, l, m_l, and m_s.

n is the principal energy level
$\boldsymbol{l}$ describes the shape of the orbital
$\mathbf{m}_l$ describes the orientation of the orbital and
$\mathbf{m_s}$ indicated the spin of the electron.

Further, as ***n*** gets larger more orbital shapes ($\boldsymbol{l}$'s) become available and as more shapes become available, those shapes have more possible orientations ($\mathbf{m}_l$'s).

Image derived from 1https://en.wikipedia.org/wiki/Atom#/media/File:Helium_atom_QM.svg

The H atom's only electron:

n = 1, $l = 0$, $m_l = 0$, and $m_s = 1/2$

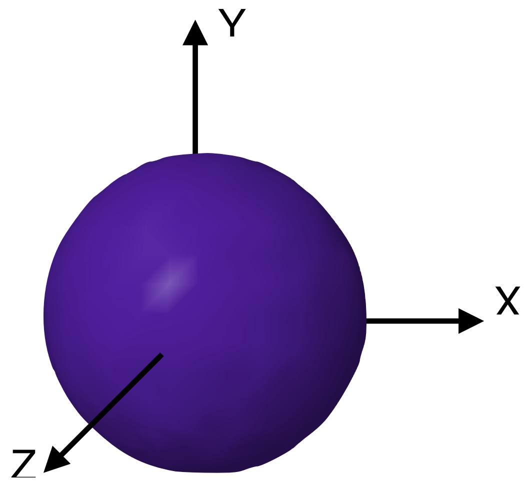
He's two e^-'s:

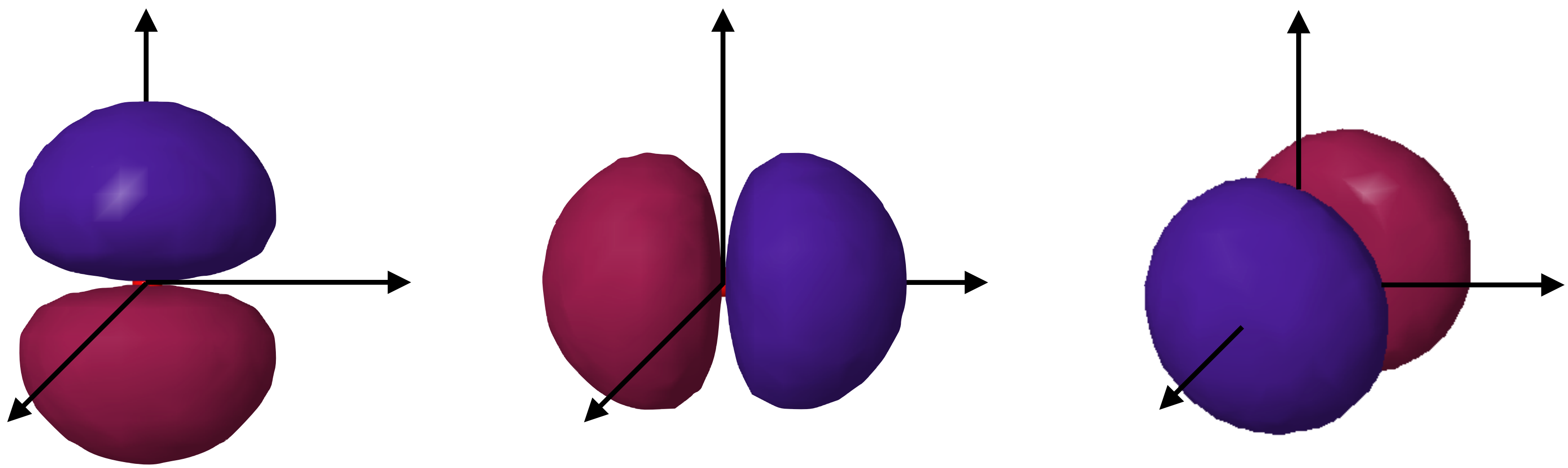
n = 1, $l = 0$, $m_l = 0$, and $m_s = 1/2$
n = 1, $l = 0$, $m_l = 0$, and $m_s = -1/2$

B's five e^-'s:

n = 1, $l = 0$, $m_l = 0$, and $m_s = 1/2$
n = 1, $l = 0$, $m_l = 0$, and $m_s = -1/2$
n = 2, $l = 0$, $m_l = 0$, and $m_s = 1/2$
n = 2, $l = 0$, $m_l = 0$, and $m_s = -1/2$
n = 2, $l = 1$, $m_l = 1$, and $m_s = 1/2$

Models


Y
X
Z



Use the periodic table to determine electron configurations

Use the periodic table to determine the number of valence electrons

Use the periodic table to identify metals and non-metals

Use the periodic table to remember trends in size

Use the periodic table to remember trends in electronegativity

Use the periodic table to predict likely charges of ions

Use the periodic table to predict likely bond formation

Use trends in size, electron configuration, and nuclear charge to explain electronegativity trend

Introduce Valence Bond Theory (hybridization)

The Periodic Table Is Your Friend

Sections 1.1 – 1.3

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
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Remember how electrons are distributed/electron configuration
Remember the importance of valence electrons/the valence shell

C electron config
and # of valence e⁻’s?

	s^1	s^2											p^1	p^2	p^3	p^4	p^5	p^6
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
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5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og

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Br electron config
and # of valence e⁻'s?

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Identify metals and non-metals

The Periodic Table Is Your Friend: Metals tend to gain and nonmetals tend to lose electrons

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Na $1s^2\ 2s^2\ 2p^6\ 3s^1$

F $1s^2\ 2s^2\ 2p^5$

Why

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Different Ways of Representing Chemicals

The Periodic Table Is Your Friend

Review

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Identify metals and non-metals

The Periodic Table Is Your Friend: Size

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Remember periodic trends

The Periodic Table Is Your Friend: Electronegativity

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Remember periodic trends

Why does electronegativity or the size of the atom matter?

High energy electrons are reactive

low energy electrons are less reactive

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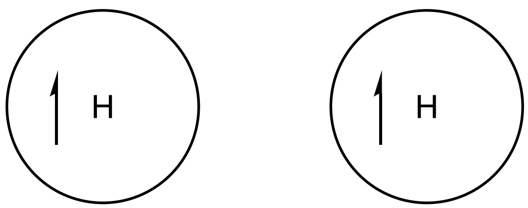
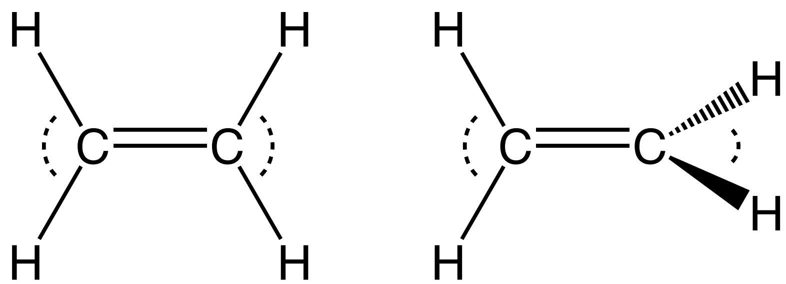
Predict the number of electrons or bonds needed for an element to form a stable compound

H—H



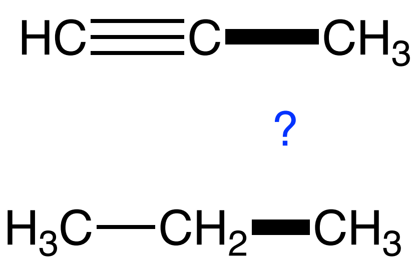
Wait, what can we use Valance Bond Theory for?



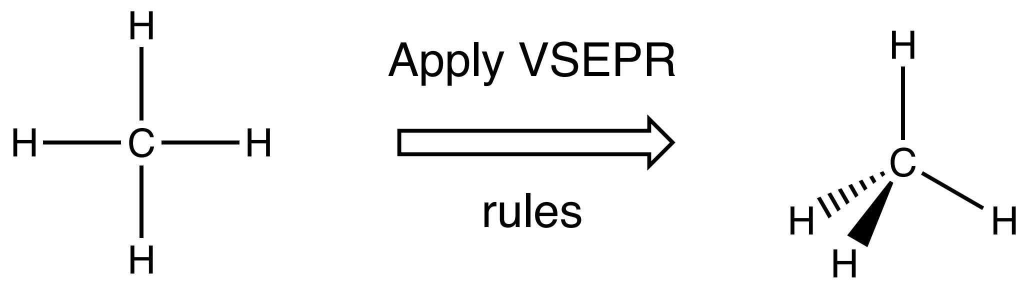
Which one? Both C atoms are trigonal planar

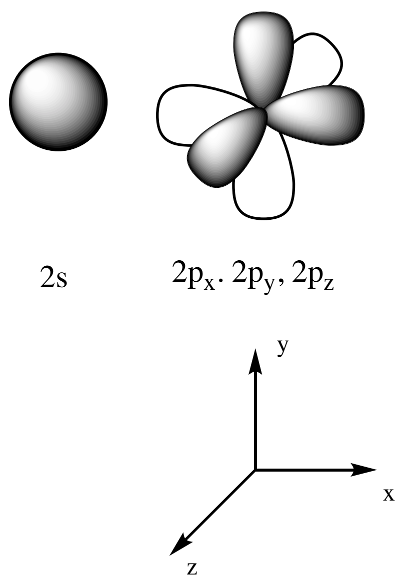
Why is there free rotation around C to C single bonds but not C to C double bonds?

Which bond is stronger?

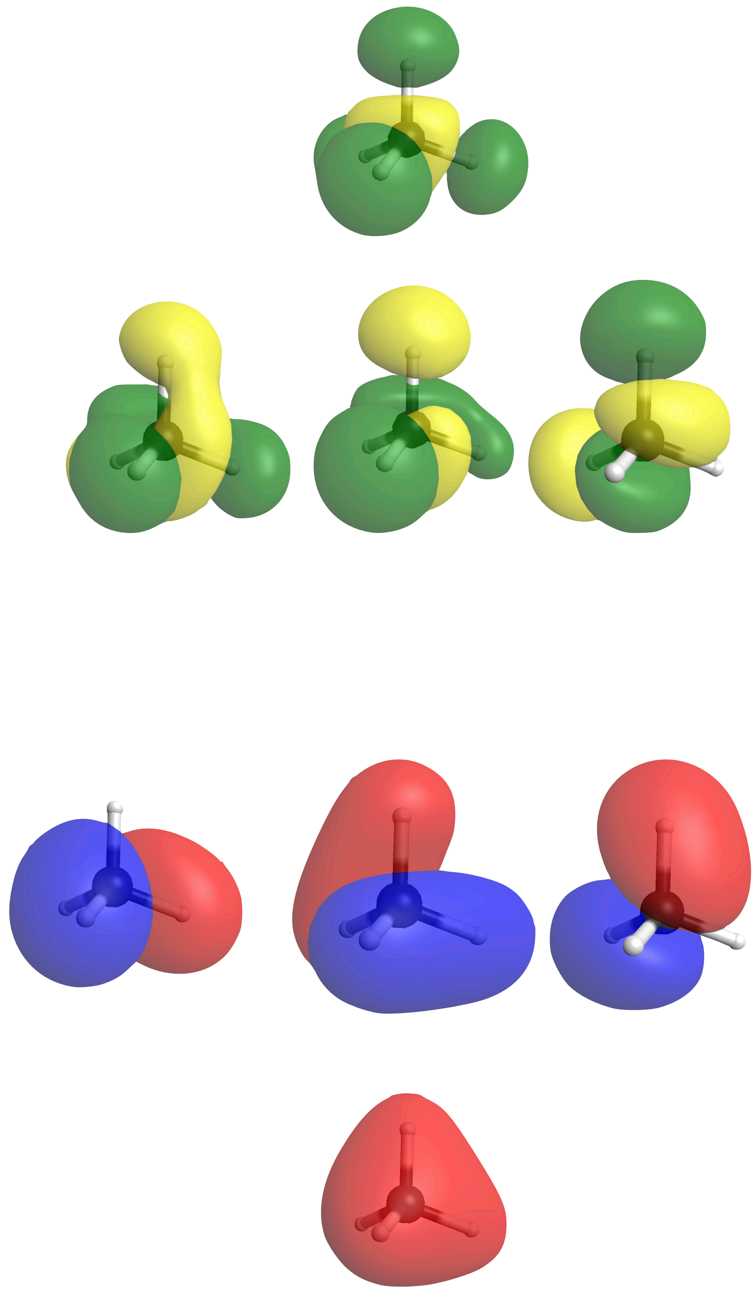


Explain observations and make predictions based on Valence Bond Theory


H
H
C
H
H
Apply VSEPR
rules
H
C
H
H
H


2s
2px. 2py, 2pz
y
x
z

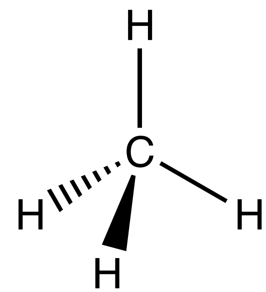
Just a Reminder that what I just said about orbitals being the "wrong" shape isn't a problem in MO theory

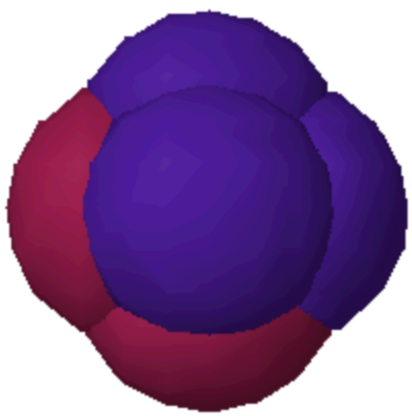


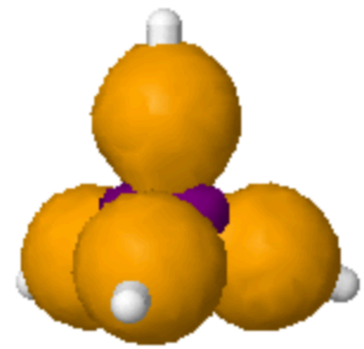
one 2s orbital
and
three 2p orbitals
from
one C atom

four 1s orbitals
from
four H atoms

https://www.westfield.ma.edu/cmasi/organic/hybrid/hybrid.html

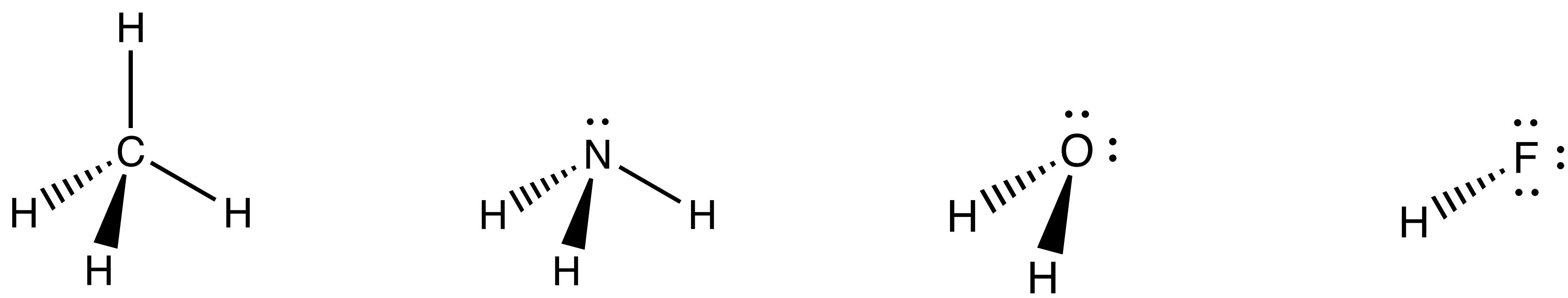






https://www.westfield.ma.edu/PersonalPages/cmasi/organic/hybrid/hybrid.html

Identify atoms that use sp^3 hybrid orbitals to form bonds and hold lone-pair electrons



Identify atoms that use sp^3 hybrid orbitals to form bonds and hold lone-pair electrons

- hybrid orbitals are used to form σ bonds and to hold lone-pair electrons
- in the valence bond model, single bonds are always σ bonds
- double and triple bonds are formed from σ bonds plus π bonds

How to determine hybridization:

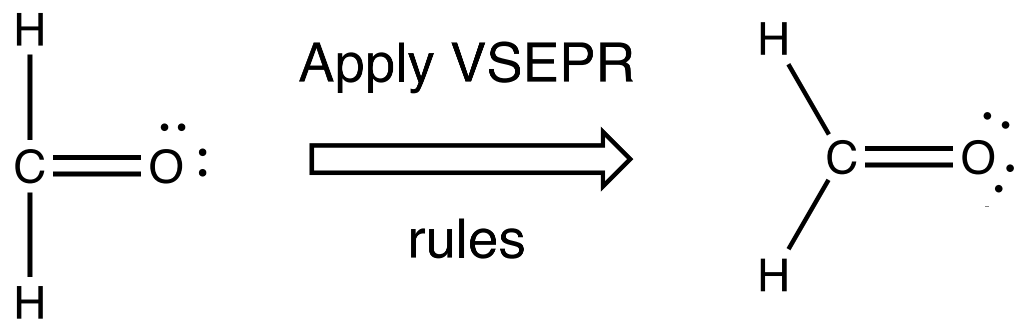
# of hybrid orbitals needed = # of σ bonds + pairs of lone-pair electrons

or

# of hybrid orbitals needed = # number of directions electrons must be pointed in

count out the # of atomic orbitals need to make the hybrid orbitals
starting with the 2s orbital (or 3s if appropriate)

name the hybrid orbitals sp^n where n is the number of p orbitals used



https://www.westfield.ma.edu/cmasi/organic/hybrid/hybrid2.html

Identify atoms that use hybrid orbitals to form bonds and hold lone-pair electrons

Triple bonds and sp$^?$ hybridization

Sections 1.5 - 1.10

https://www.westfield.ma.edu/PersonalPages/cmasi/organic/hybrid/hybrid2.html

Identify atoms that use hybrid orbitals to form bonds and hold lone-pair electrons

The methyl cation, anion, and radical

Sections 1.5 - 1.10

CH_3^+ CH_3^- $CH_3^\bullet$

Determine the hybridization of unusual molecular fragments

Practice: Determine the Hybridization of the Atoms in the Following Molecules

of HO's Needed

σ bonds + # pairs of lone-pair e⁻'s

count out # of AO's needed

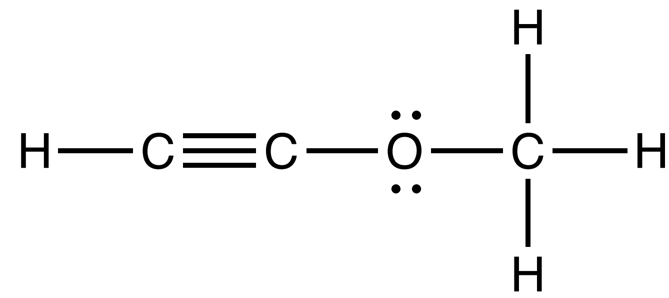
2s x 2p x etc

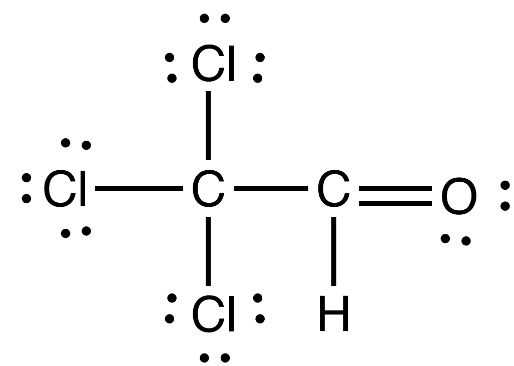
name the hybrids

sp^3 made from one s and three p orbitals

sp^2 made from one s and two p orbitals

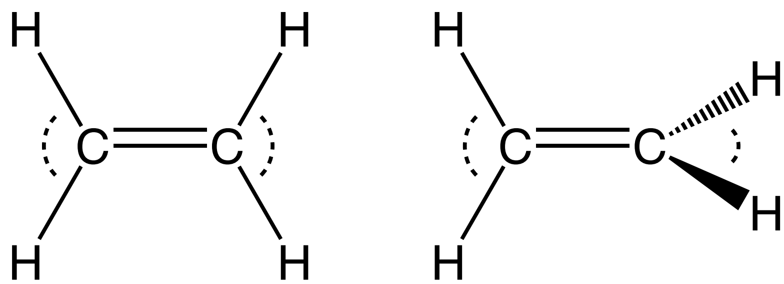
sp made from one s and one p orbital





$N{\equiv}C-CH_2-NH_2$

What can we use Valance Bond Theory for?



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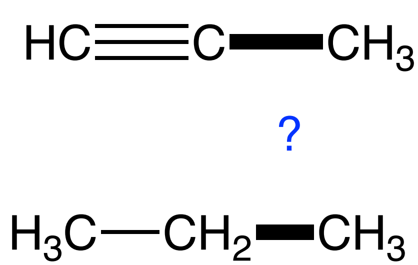
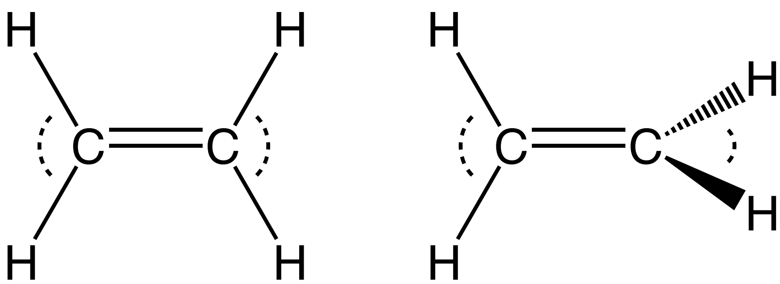
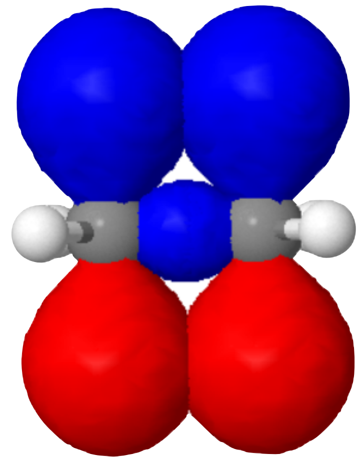
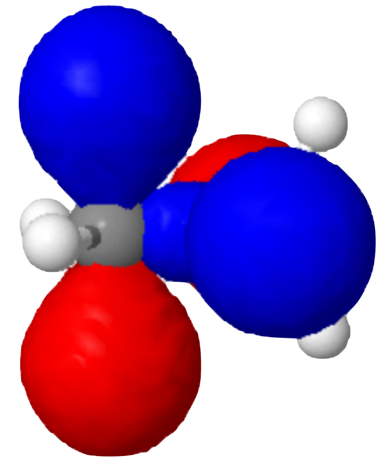


Explain observations and make predictions based on the hybridization of an atom

What can we use Valance Bond Theory for?







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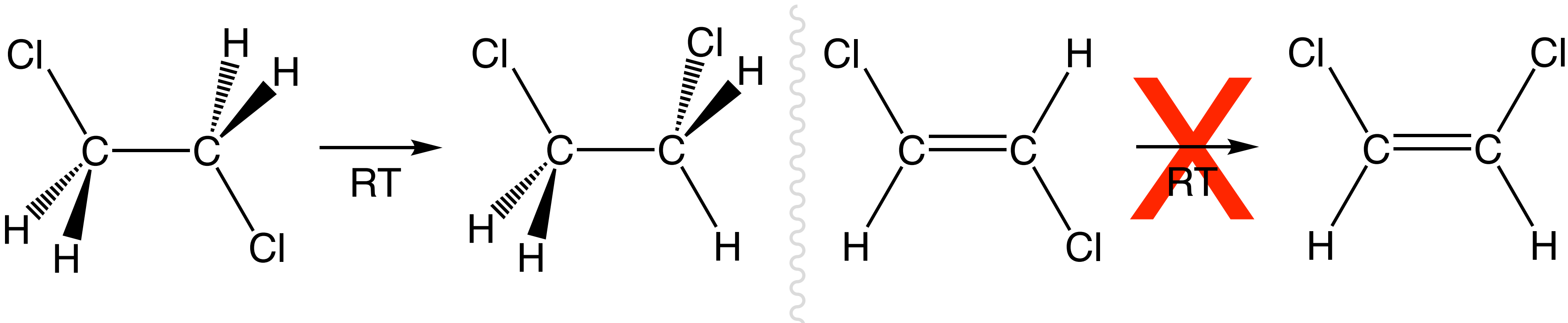
Explain observations and make predictions based on the hybridization of an atom

What can we use Valance Bond Theory for?

Why is there free rotation around C to C single bonds but not C to C double bonds?

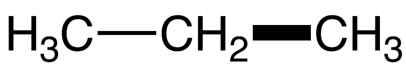


Explain observations and make predictions based on the hybridization of an atom

What can we use Valance Bond Theory for?

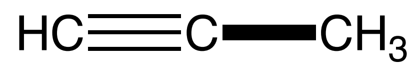
Which bond is strongest?

370 kJ/mol[2], 355±8 kJ/mol[3]



426 kJ/mol[1]

490 kJ/mol[4]



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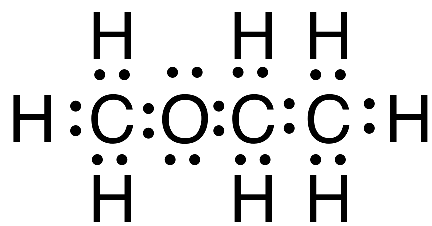
[2] Organic Chemistry, 10th ed. McMurry.

[3] Chem. Rev. **66**, 465 (1966).

[4] J.Chem.Ed. **42**, 502 (1965)



Chemists use different drawings to place emphasis on different aspects of a molecule.

Representations are used to solve typographical issues.

Molecular Formulas as Compared to Condensed Structures/Structural Formulas

In organic, molecular formulas are written C_xH_y(and other elements listed alphabetically)

For example:

C_3H_8O C_3H_7ClO

Molecular Formulas as Compared to Condensed Structures/Structural Formulas

In organic, condensed structures typically start with a C, and everything immediately to the right of the C is connected to that first C. When the the first C is finally connected to the second C, now that atoms right of the second C are connected to second C. In acyclic unbranched molecules atoms to the right of the second C are not connected to the first C.

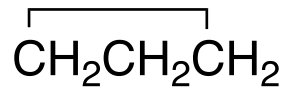
C_3H_8O $CH_3CH_2OCH_3$ $CH_3CH_2CH_2OH$ $CH_3CHOHCH_3$

In organic, condensed structures typically start with a C, and everything immediately to the right of the C is connected to that first C. When the first C is finally connected to the second C now that atoms right of the second C are connected to second C. In acyclic unbranched molecules, atoms to the right of the second C are not connected to the first C.

CH_2CHCH_3

Because bonds are not drawn, condensed structures require the reader to bring some chemical knowledge to their interpretation.

Condensed Structures/Structural Formulas: Cyclic Molecules



$CH_3CH(OH)CH_2CH_3$ $CH_3(CH_2)_3CH_3$ $CH_3CH_2CH(CH_3)_2$

Parentheses **( )** in structures are typically used to set off side chains, to indicate a repeating unit, or to indicate multiple groups of the same structure.

Often, chemists omit parentheses when they are not absolutely necessary,

$CH_3(CH_2)_3CH_3$

$CH_3CHOHCH_3$

$CH_3CH(OH)CH_3$

$CH_3COCH_2CH_3$

$CH_3C(O)CH_2CH_3$

and sometimes chemists do things for aesthetic reasons.

$C(CH_3)_3OH$ $CH_3C(CH_3)_2OH$ $(CH_3)_3COH$

Convert Condensed Structures to Kekulé Structures

$CH_3CHOHCH_2CH_3$

$CH_3C(O)CH(CH_3)_2$

When a bond ends and the atom isn't labeled it is assumed to be C.

When there aren't enough bonds drawn to a C atom, the "missing" bonds are C atom to H atom bonds.

All other atoms are labeled.

Heptane $CH_3CH_2CH_2CH_2CH_2CH_2CH_3$

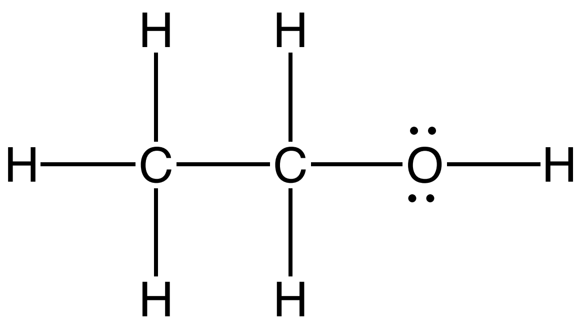
2-heptanol $CH_3CHOH(CH_2)_4CH_3$

Different structures serve different purposes, but they represent the same things

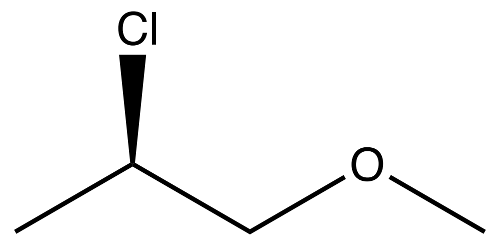
Converting Between Structure Types

Sections 1.12

convert Lewis to skeletal



convert skeletal to condensed



convert structural formula to skeletal

$CH_3CH(OH)CH_2CH(CH_3)CH_2CH_3$

convert skeletal to condensed