(2) **Today**

Reviewing Periodic Trends

Section 1.4
Introduction to Chemical Bonding Theories
octet rule etc

Sections 1.5-1.10
Valence Bond Theory

Next Class (3)

Sections 1.5-1.10
Valence Bond Theory

Skipping Section 1.11 for now
An introduction to Molecular Orbital Theory

Sections 1.12
Drawing Chemical Structures

(4) **Second Class from Today**

Sections 2.1 - 2.4
Polar Covalent Bonds, Formal Charges,
Resonance/Electron Delocalization

Sections 2.4 – 2.6
Resonance/Electron Delocalization

Third Class from Today (5)

Sections 2.7 – 2.11
Acids and Bases

Today's outline sent to campus email moments ago

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)

Different Ways of Representing Chemicals

The Periodic Table Is Your Friend

metals tend to lose e⁻ when reacting with nonmetals

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
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
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
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

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

we will mostly talk about molecules made from these elements

nonmetals tend to gain or share e⁻'s

Identify metals and non-metals

The Periodic Table Is Your Friend: Size

Review

Li vs F which occupies more volume? Li

e⁻'s occupy the volume ... not the protons + neutrons

F^{9+} $2e^-$ } e^-

Li^{+3} $2e^-$ } e^-

Li's valence e⁻'s are in the n=2 shell ... experience a lower effective nuclear charge than the e⁻'s in F's n=2 shell

F's valence e⁻'s are in the n=2 shell

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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

atomic radius increases in the indicated direction

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Sizes in a given row aren't that different ... so this size difference is not particularly important

Size in different rows are very different and these differences have significant effects on reactivity

Remember periodic trends

The Periodic Table Is Your Friend: Electronegativity

The ability of an atom to draw e⁻'s in a bond toward itself

F is more eneg than O because ... the e⁻'s in the bond to F experience a higher effective nuclear charge than e⁻'s in a bond to O

experience

increases in the indicated direction

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weird stuff happens here

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
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Why is Cl less eneg than F? e⁻'s in a bond to Cl are in Cl's n=3 shell which is farther from the nucleus. Greater distance = less attraction

Remember periodic trends

Why does electronegativity or the size of the atom matter?

$$E = k \frac{q_1^- q_2^+}{r}$$

Review

High energy electrons are reactive

e⁻'s that experience a low effective nuclear charge are higher in E... more reactive

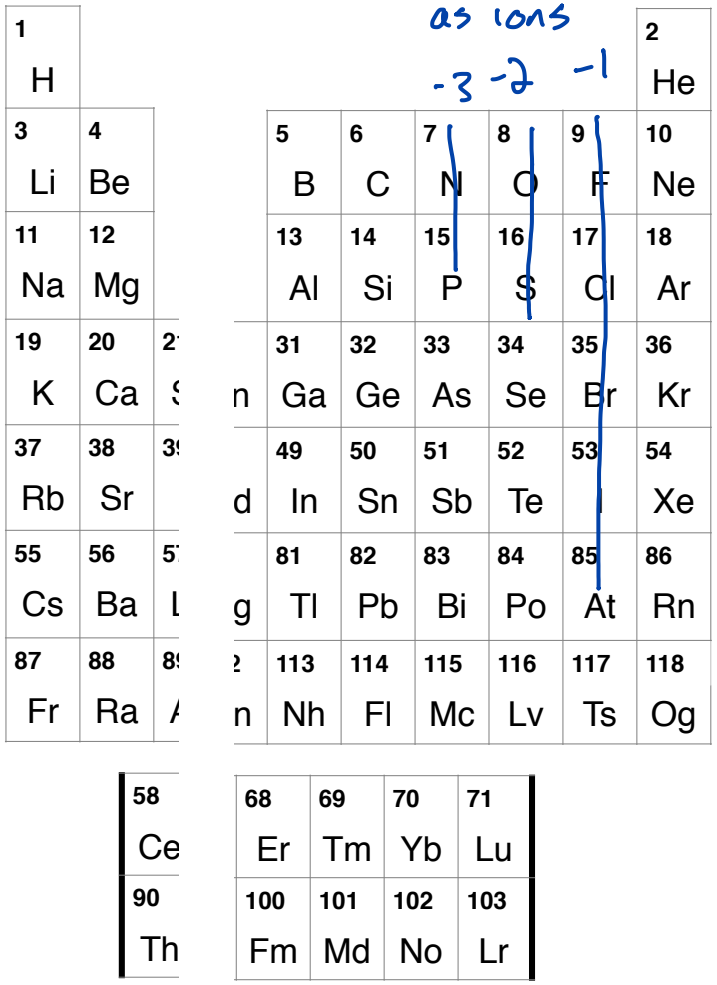
e⁻'s that are concentrated are attractive

low energy electrons are less reactive

e⁻'s that experience a high effective nuclear charge are lower in E... less reactive

e⁻ spread out over a larger volume are less reactive because they are less attractive

concentrated charge is attractive analogous to how a $100 bill is more attractive than 100,000 pennies spread across the floor



H 1 bond

F 1 bond (also Cl, Br, I)

O 2 bonds ... but can do 3 + 1 (normal, reactive)

N 3 bonds ... can do 4 + 2

C 4 bonds!

reactive intermediates with 3 bonds exist

very few stable molecules/compounds where C has 3 bonds come to mind

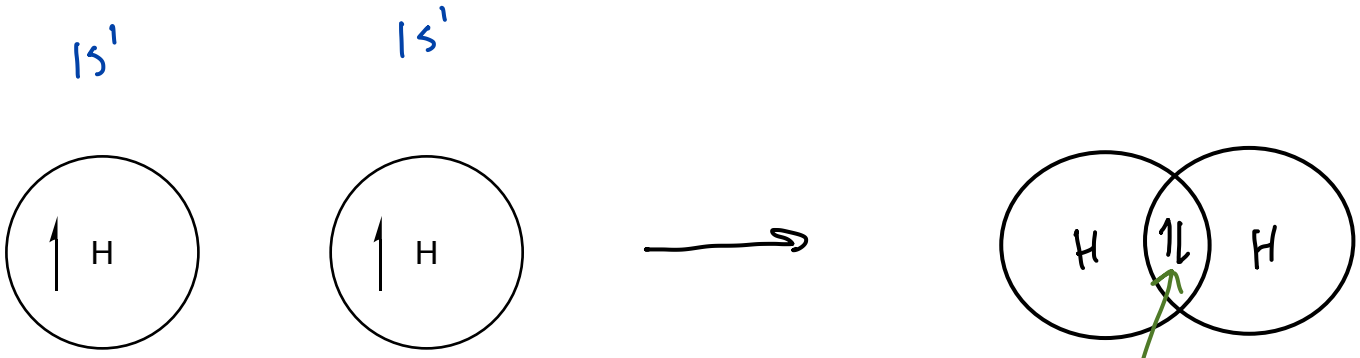
$C{\equiv}O$ $Na^{+}\,{}^{-}C{\equiv}N$ $Ca^{2+}[C{\equiv}C]^{2-}$

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

Overlapping Atomic orbitals can share e⁻'s

e⁻'s shared in this way experience more ⊕ and are lower in E

H—H

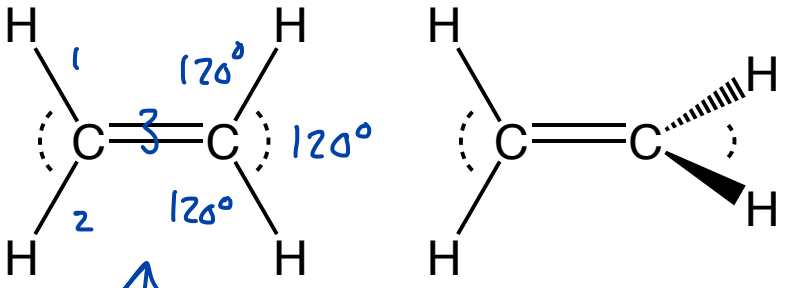


overlap occurs between two half-filled orbitals or between a filled orbital + an empty orbital or in reative intermediates between a half-filled orbital and an empty orbital

both e⁻'s now get to experience more ⊕ charge

mutual attraction for a pair of e⁻'s

Wait, what can we use Valance Bond Theory for?



Which one? Both C atoms are trigonal planar

this one

— means in the plane of the paper

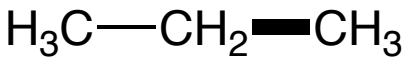
◢ means coming out of plane towards the viewer

||||| means going out of plane away from the viewer

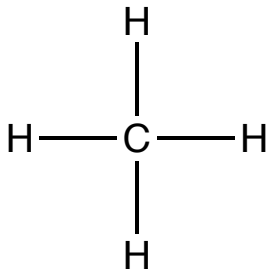
Why is there free rotation around C to C single bonds but not C to C double bonds?

Which bond is stronger?

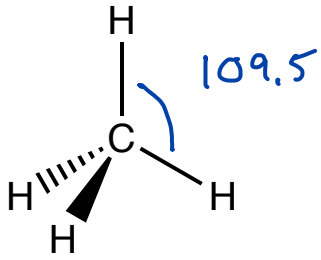
?

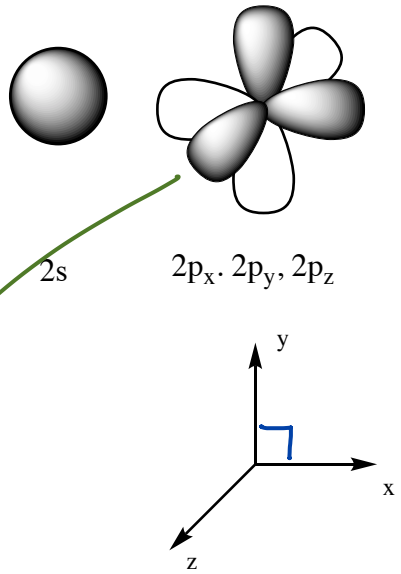


Explain observations and make predictions based on Valence Bond Theory



Apply VSEPR rules





these orbitals are not pointed in the "right" direction

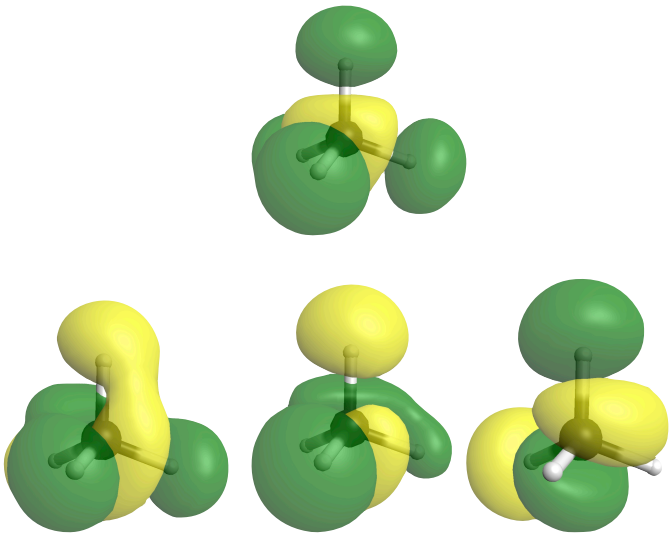
4 H atoms $1s^1$ $1s^1$ $1s^1$ $1s^1$

1 C atom $2s^2 2p_x^1 2p_y^1 2p_z$

$2s^2 2p^2$ not $2s^2 \cancel{2p_x^2} 2p_y 2p_z$

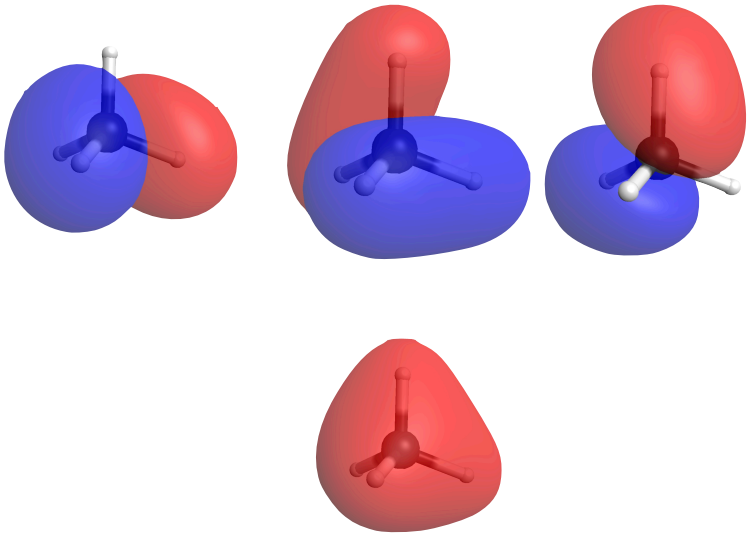
e^-'s would repel each other

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

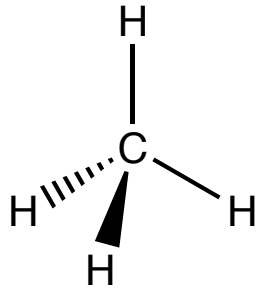


one 2s orbital
and
three 2p orbitals
from
one C atom

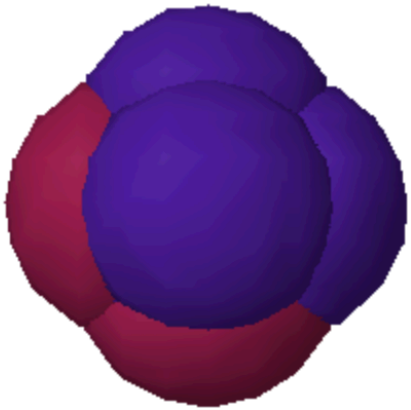
four 1s orbitals
from
four H atoms

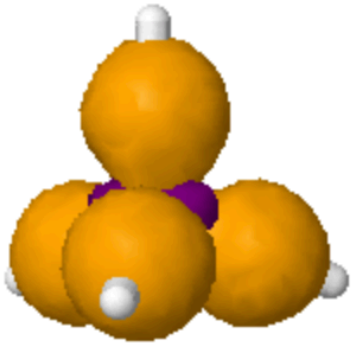


https://www.westfield.ma.edu/cmasi/organic/hybrid/hybrid.html



4 go in ⟹ 4 come out





none

$2s, 2p_x, 2p_y, 2p_z$ not the correct orientation

mix to create hybrids ⟹

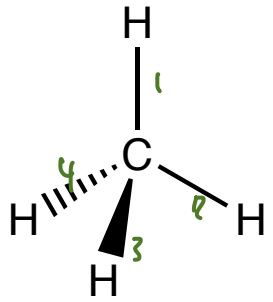
one part s

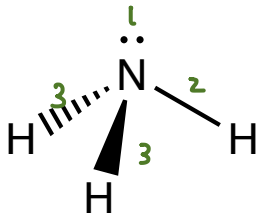
sp^3, sp^3, sp^3, sp^3

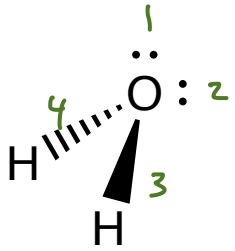
3 parts p

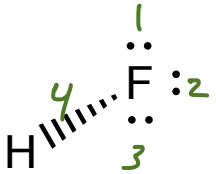
https://www.westfield.ma.edu/PersonalPages/cmasi/organic/hybrid/hybrid.html

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









VSEPR

tetrahedral

tetrahedral arrangement of e^-

tetrahedral arrangement of e^-

tetrahedral arrangement of e^-

Four sp^3 hybrids on C

Four sp^3 hybrids on N

3 for bonds

1 for lp e⁻'s

4 sp^3 HOs

2 for bonds

2 for lp e⁻

4 sp^3 HOs

1 for the bond

3 for the lp e⁻

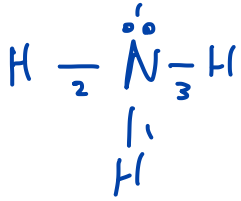
there is disagreement as to whether hybridization is necessary for these 2

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

single bonds are σ bonds

- 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

4 = 3 + 1 or

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

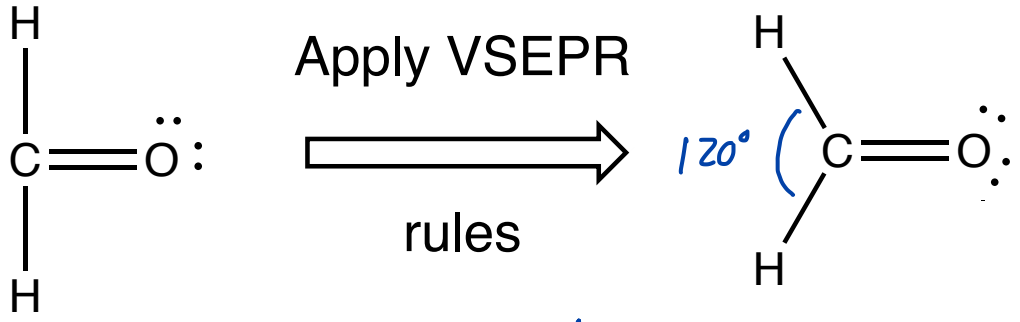
need to mix 4 AO's to make 4 HO's

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

$2s \times 2p_x \times 2p_y \times 2p_z \Longrightarrow$ four sp^3

↑ 1 parts ↖ 3 parts p



C atom 3 σ bonds 3 HO's needed

$2s \times 2p_x \times 2p_y \Rightarrow sp^2, sp^2, sp^2$

O atom 1 σ bond + 2 pair of lp e⁻'s 3 HO's needed

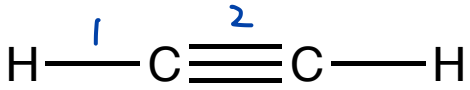
$2s \times 2p_x \times 2p_y \Rightarrow 3$ sp^2 hybrids

1st bond of db is a σ bond made by overlapping a C's sp^2 with an O's sp^2

2nd bond of db is a π bond made by overlapping unhybridized $2p_z$ orbitals

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

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



How many HO's needed? # of groups of e⁻'s or # of σ bonds & pairs of lp e⁻

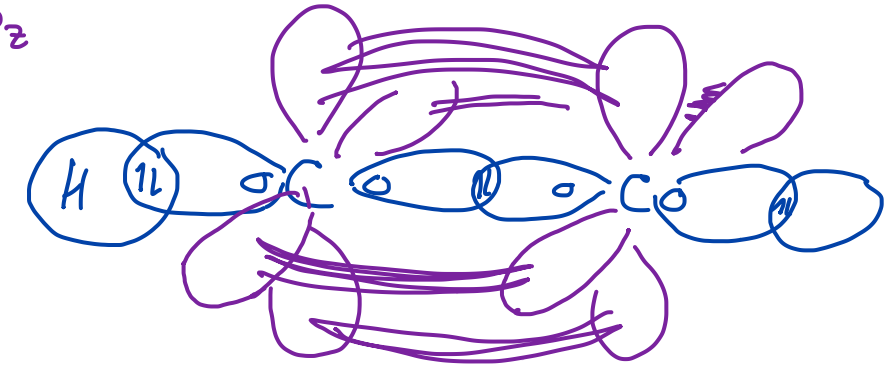
2

2 σ bonds

2 HO's needed (on each C atom)

2s + $2p_x$ => sp, sp

$2p_y$ + $2p_z$



$2p_y$ on left C overlaps with $2p_y$ on right C ... π bond

$2p_z$ on left overlaps with $2p_z$ on right 2nd π bond

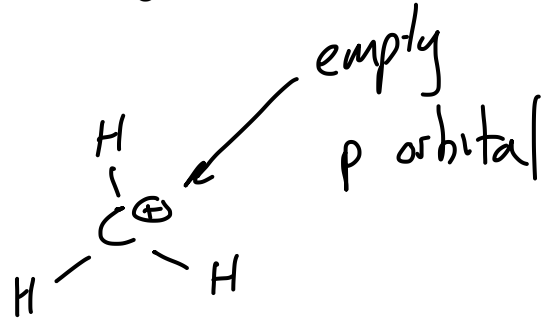
https://www.westfield.ma.edu/PersonalPages/cmasi/organic/hybrid/hybrid2.html

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

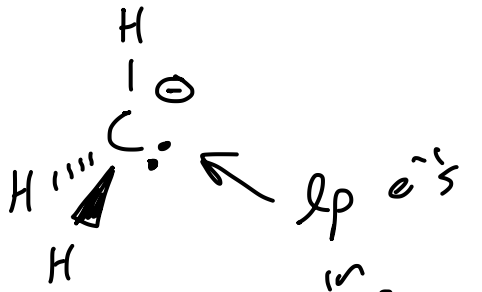
CH_3^+



3 HO's

sp^2

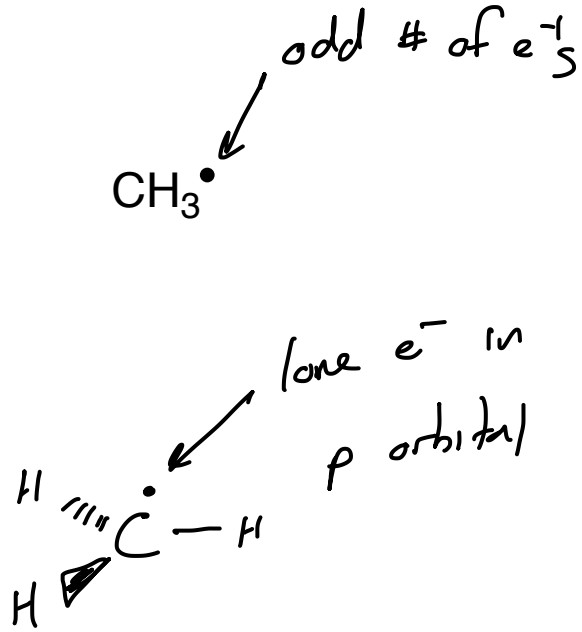
CH_3^-



4 HO's

sp^3

$CH_3^{\bullet}$



3 HO's

sp^2

Determine the hybridization of unusual molecular fragments

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