LEC (3) CHEM 30A Jan 12th

(1) SHAPES OF MOLECULES
(2) DRAWING ORGANIC STRUCTURES
(3) RESONANCE

HMK: Read rest of Ch 1
Problems 1.14–1.17, 1.48–1.54

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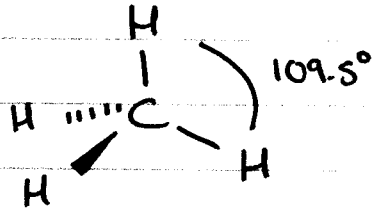
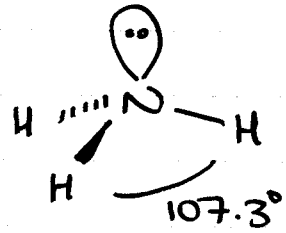
(1) SHAPES OF MOLECULES

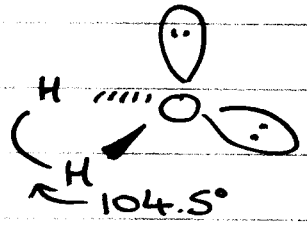
– PAIRS OF ELECTRONS IN VALENCE SHELL
(BONDED & NONBONDED – lone pairs)



TETRAHEDRAL



PYRAMIDAL



BENT

<u>BUT</u> GEOMETRY AROUND C, N, O is STILL DESCRIBED AS TETRAHEDRAL

REPULSION LP-LP > LP-BP > BP-BP

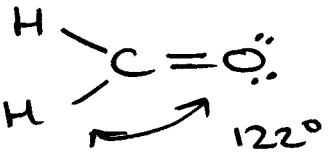
ADD # BP to LP
(or # atoms) to LP

2 LINEAR
3 TRIGONAL PLANAR
4 TETRAHEDRAL
5 TRIGONAL BIPYRAMIDAL
6 OCTAHEDRAL

ALSO:
TREAT MULTIPLE BONDS AS SINGLE BONDS

So, CO_2 $O=C=O$ LINEAR

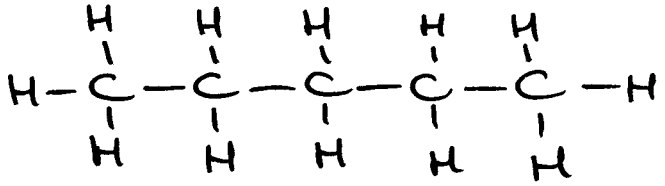
$H-C\equiv C-H$ LINEAR



TRIGONAL PLANAR

$A\equiv B > A=B > A-B$

(2) DRAWING ORGANIC STRUCTURES



PENTANE
(structural formula)

- Condensed formula

$CH_3CH_2CH_2CH_2CH_3$ $CH_3(CH_2)_3CH_3$

- line formula

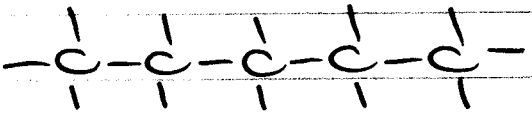
- draw chains as zigzags
- leave out H attached to C
- draw lone pairs

a) 

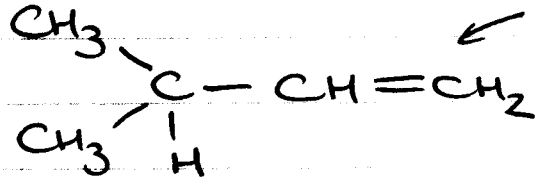
this is a C atom with 2 Hs on it

this is a C atom with 3 Hs on it

DO NOT WRITE

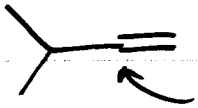
C-C-C-C-C or 

b) $(CH_3)_2CHCHCH_2$?

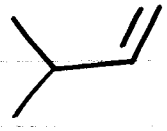


← what's missing?

maybe you would draw this:

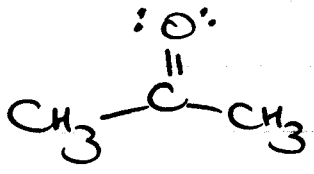
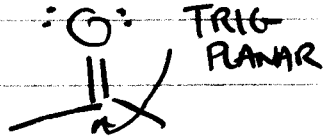


← geometry of C atom? => TRIGONAL PLANAR

So 

Try to be as true to molecular shape as possible.

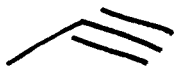
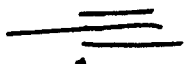
e.g.

c) $CH_3(CO)CH_3$ =>  => 

TRIG PLANAR

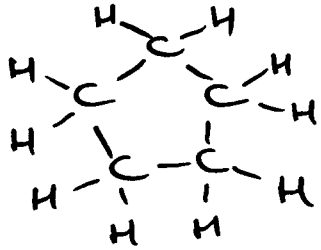
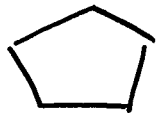
not 

d) $CH_3CCH \Rightarrow CH_3-C\equiv C-H$

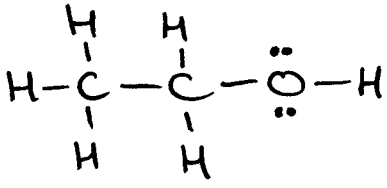
not  but 

↑ linear

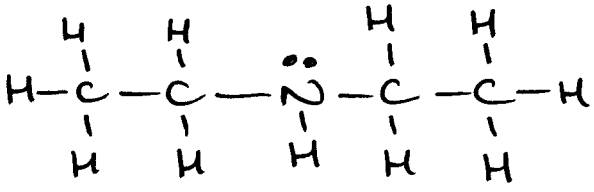
- RINGS

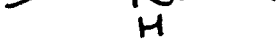
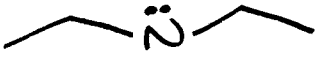
 ≡  ← each of these is a CH_2

- HETEROATOMS
(DRAW Hs on them)

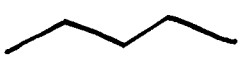


 not



 not 

- Example C_5H_{12}

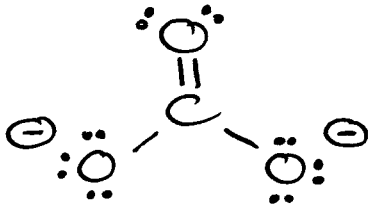
  

CONSTITUTIONAL ISOMERS

Same formula, different arrangements of atoms

③ RESONANCE

consider CO_3^{2-}

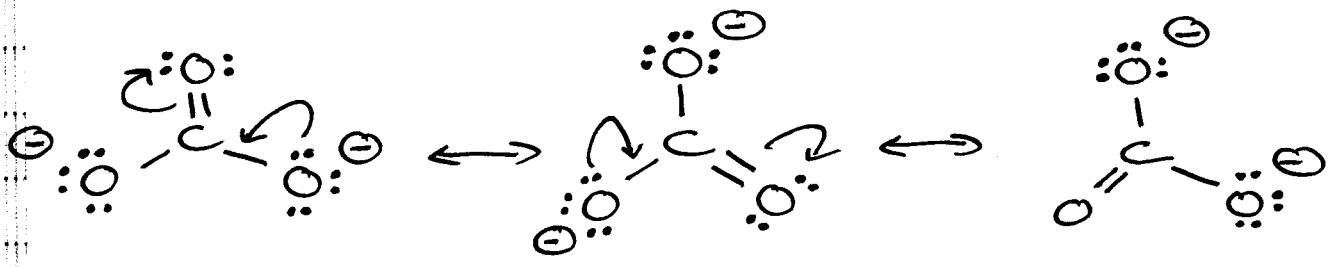


one C=O BOND
two C–O BONDS

C=O shorter/stronger bond than C–O

In CO_3^{2-}, however, all carbon/oxygen bonds are identical

WHY?



RESONANCE CONTRIBUTORS (ALL EQUIVALENT)

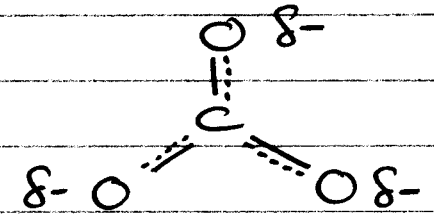
$\longleftrightarrow$ SEPARATES RESONANCE CONTRIBUTORS

ARROWS

 CURLY ARROW – movement of a pair of electrons

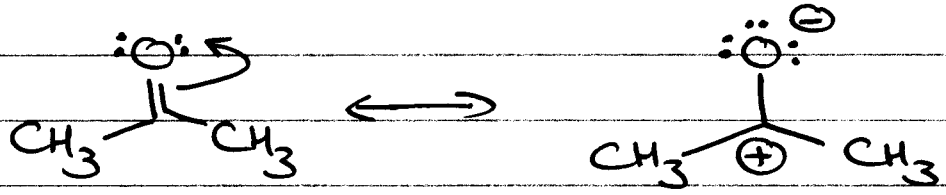
None of these contributors actually exist

actual structure is



RESONANCE HYBRID

Not all resonance contributors are necessarily equivalent, for example



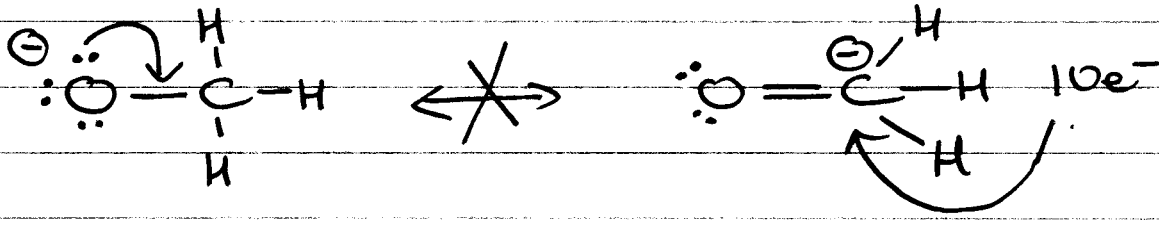
Which one of these is the most stable ?

– RULES FOR WRITING RESONANCE STRUCTURES

Do NOT

① BREAK ANY SINGLE BONDS

② VIOLATE THE OCTET RULE



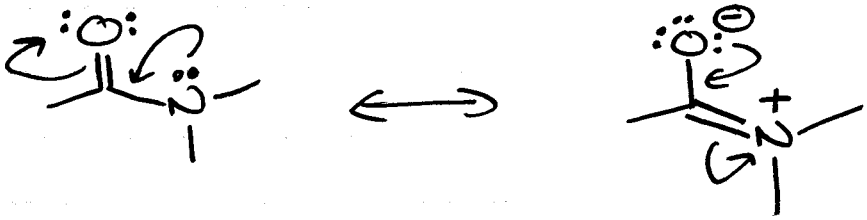
DRAWING RESONANCE STRUCTURES

Cannot break single bonds, SO we can only move electrons from double (or triple) bonds and lone pairs.

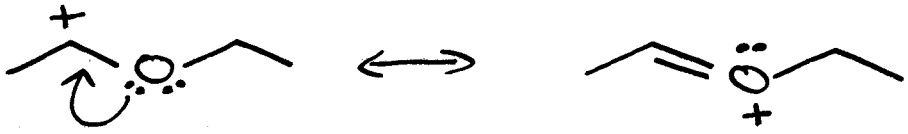
PATTERNS

(1) LONE PAIR NEXT TO π BOND (double or triple bond)

"next to" means one single bond away

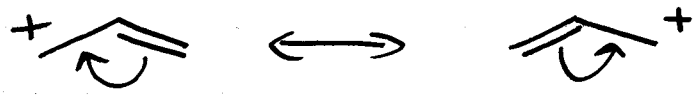


(2) LONE PAIR NEXT TO +ve CHARGE

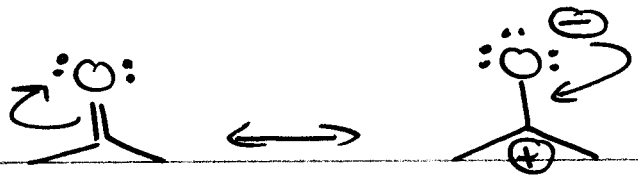


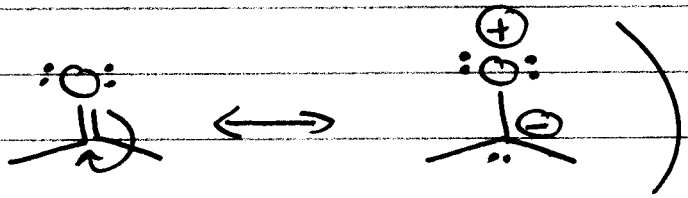
(3) π BOND NEXT TO +ve CHARGE

↷ double or triple bond

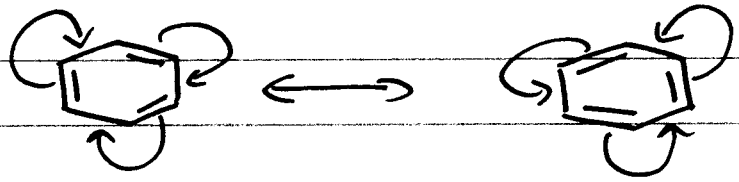


(4) π BOND BETWEEN TWO ATOMS WHERE ONE IS QUITE ELECTRONEGATIVE



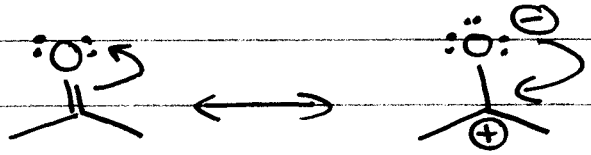
(NOT ) O is more EN than C

(5) ALTERNATING π BONDS IN A RING



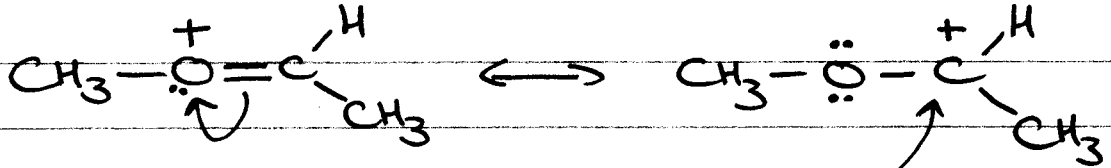
– RELATIVE IMPORTANCE OF CONTRIBUTING STRUCTURES

(1) MINIMIZE CHARGES



more significant

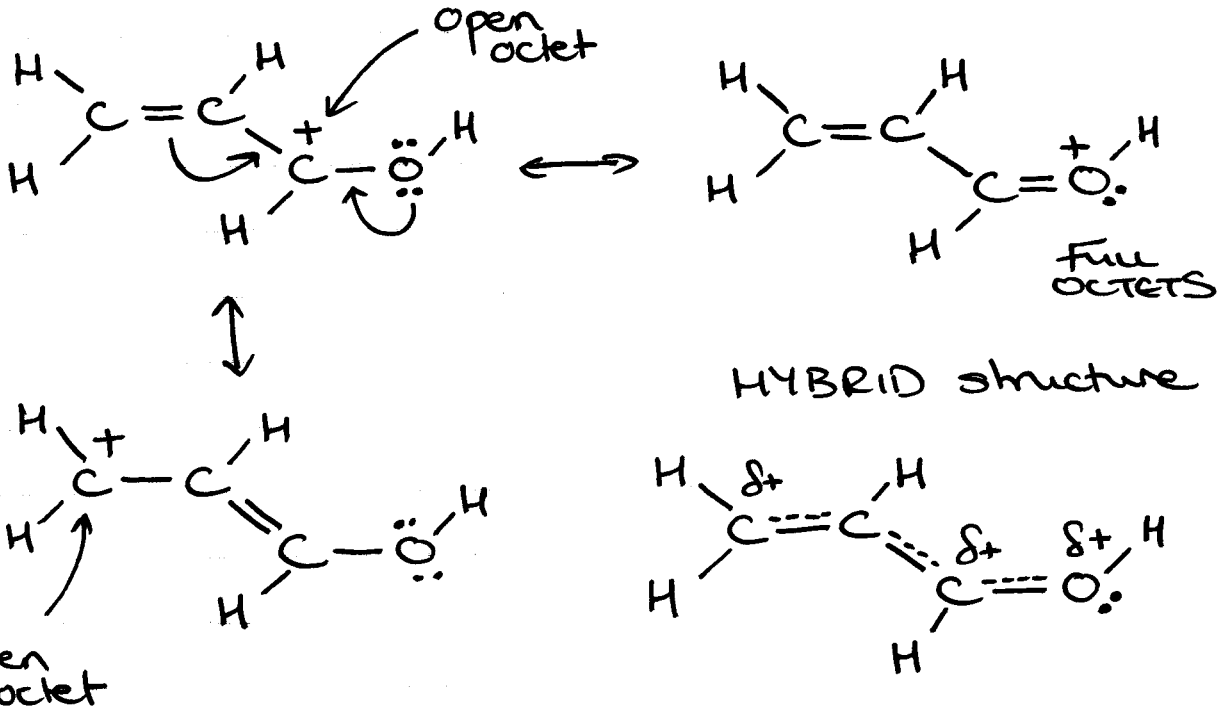
(2) MAXIMIZE OCTETS



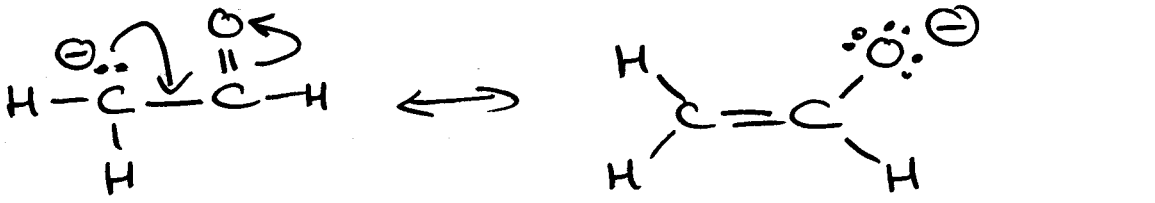
more significant

not a full octet

EXAMPLE



(3) NEGATIVE CHARGE ON MORE EN ELEMENT



next up: ATOMIC ORBITALS.