LEC 3 CHEM 30A Oct 5th

1. SHAPES OF MOLECULES
2. DRAWING ORGANIC STRUCTURES
3. RESONANCE

GRUBBS Pg 963

Hmk: READ rest of Ch 1
Problems: 1.14-1.17, 1.48-1.54 + molecular structure worksheets

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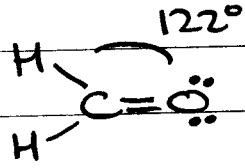
1. SHAPES OF MOLECULES

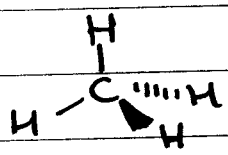
(PAIRS OF e^- IN VALENCE SHELL)
- BONDED & NONBONDED

BUT TREAT MULTIPLE BONDS AS SINGLE

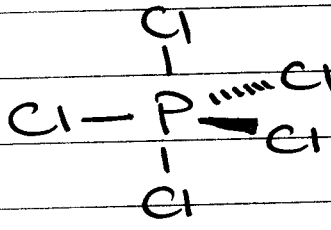
ADD #BP (or # atoms) to #LP

2 → LINEAR 

3 → TRIGONAL PLANAR 

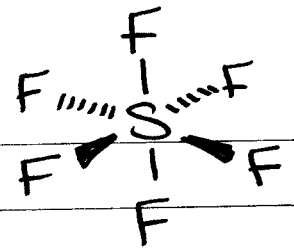
4 → TETRAHEDRAL 

, NH_3, H_2O

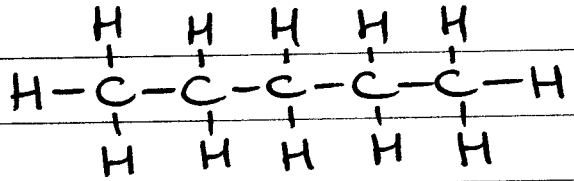
5 → TRIGONAL BIPYRAMIDAL 

PCl_5

6 → OCTAHEDRAL



(2) DRAWING ORGANIC MOLECULES

a) 

PENTANE (structural formula)

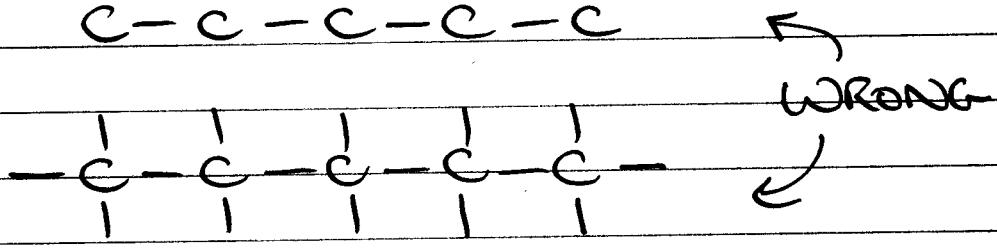
- condensed formula

$CH_3CH_2CH_2CH_2CH_3$ or $CH_3(CH_2)_3CH_3$

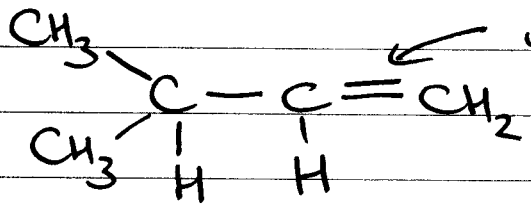
- line formula

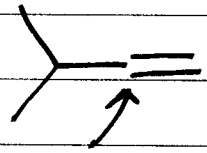
  - draw chains as ZIG-ZAGS
  - leave out any H attached to C
  - draw nonbonded electrons (lone pairs)

DO NOT WRITE

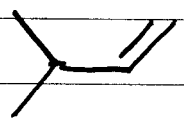


b) $(CH_3)_2CHCHCH_2$?



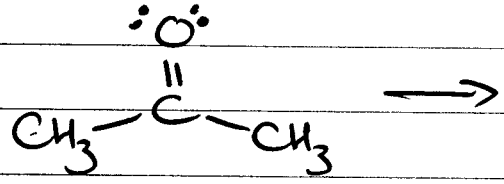
maybe you would draw 

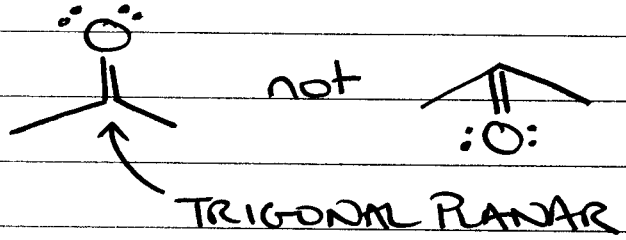
geometry of C atom
⇒ TRIGONAL PLANAR

So 

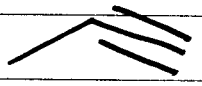
TRY to be as true to molecular shape as possible.

c) $CH_3(CO)CH_3$

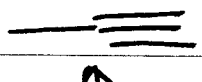




d) $CH_3CCH \Rightarrow CH_3-C\equiv C-H$

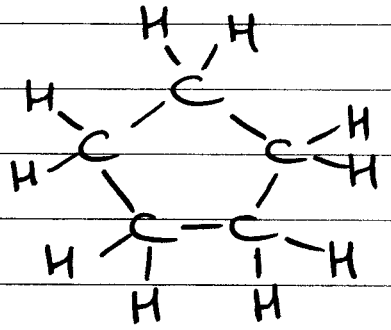


NO



LINEAR

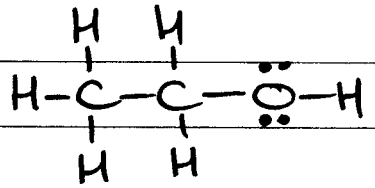
- RINGS



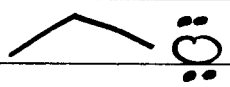
≡

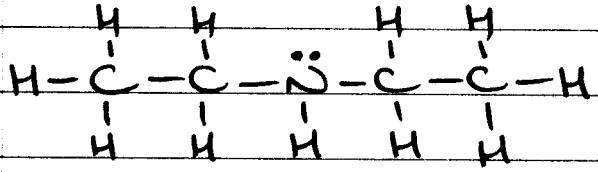
each of these is a CH_2

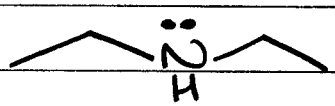
- HETEROATOMS (draw Hs & LONE PAIRS)



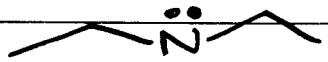
not



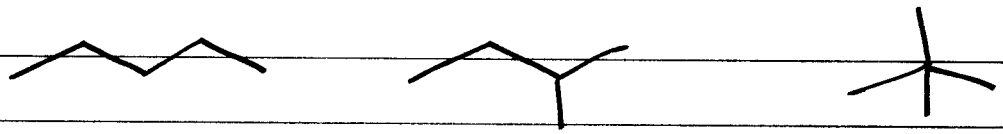




not



- example C_5H_{12}

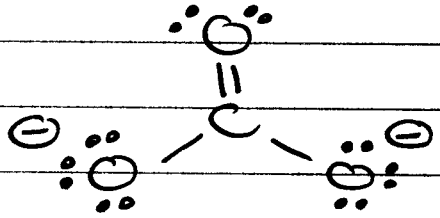


CONSTITUTIONAL ISOMERS

-same formula, different arrangements of atoms

(13) RESONANCE

consider CO_3^{2-}

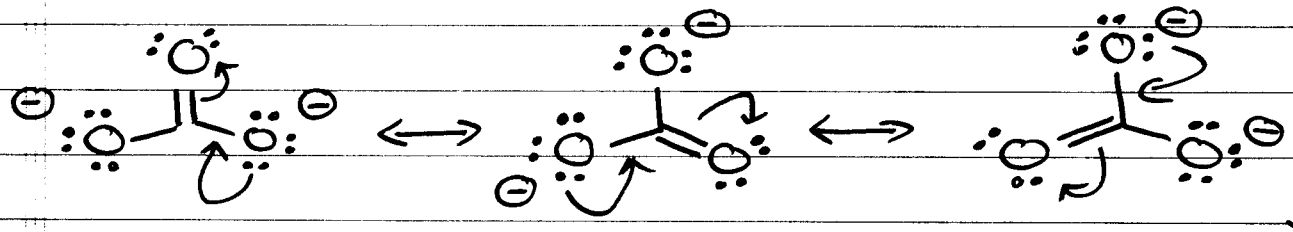


one C=O bond

two C-O bonds

C=O shorter/stronger bond than C–O

In CO_3^{2-} however, all CO bonds are identical & all angles 120° ⟹ WHY?



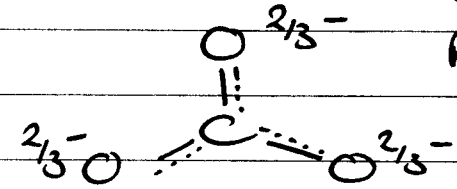
RESONANCE CONTRIBUTORS (all equivalent in this case

ARROWS ⟷ Separates resonance contributors

↷ CURLY ARROW: movement of a pair of ELECTRONS

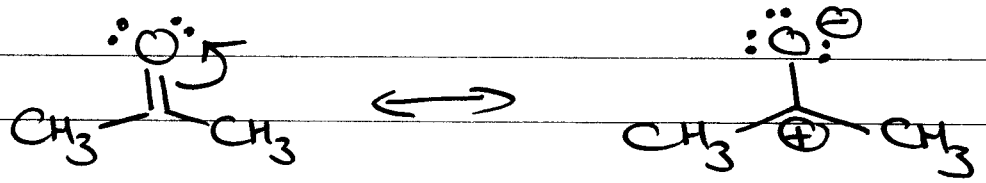
BUT NONE of these contributors actually EXIST!

actual structure is



RESONANCE HYBRID

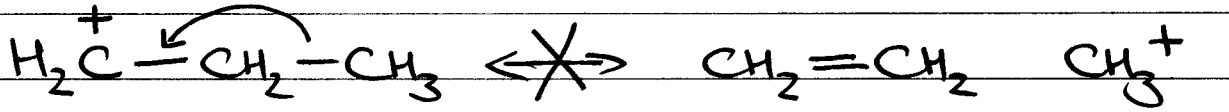
Not all resonance contributors are necessarily equivalent, e.g.



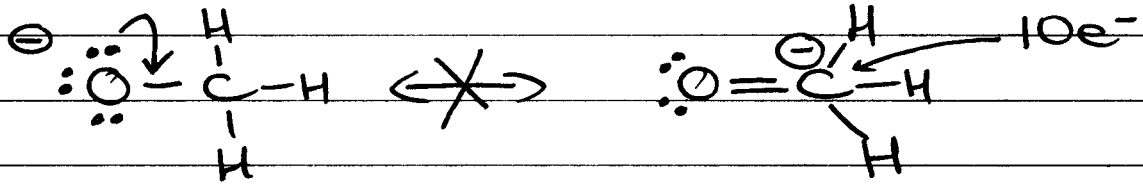
which of these is most stable?

- RULES FOR DRAWING RESONANCE STRUCTURES
- DO NOT

① Break any single bonds



② Violate the octet rule

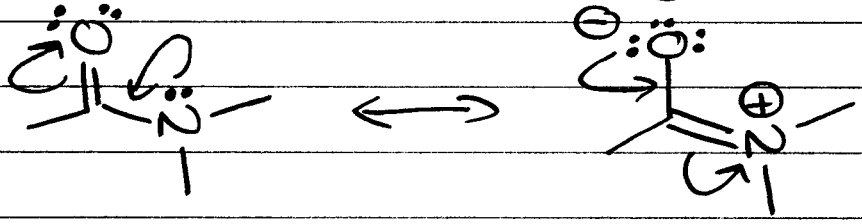


③ Move atoms (framework must stay same)

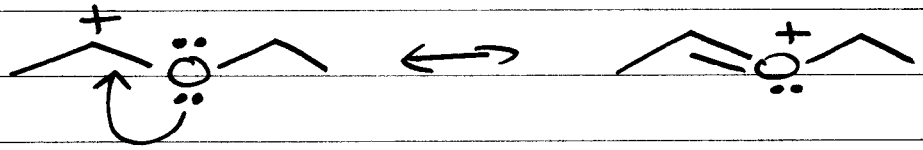
DRAWING RESONANCE STRUCTURES
- cannot break single bonds, so we can only move electrons from double (or triple) bonds and lone pairs.

PATTERNS

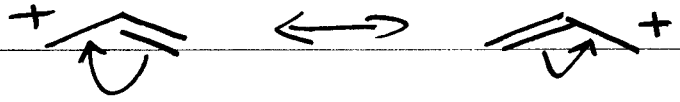
① LONE PAIR NEXT TO π BOND
double | triple
"next to" means one single bond away



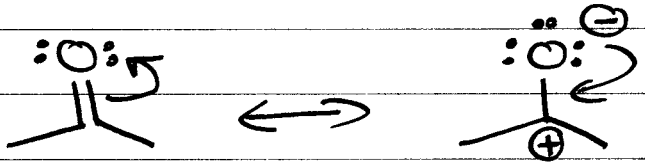
② LONE PAIR NEXT TO +VE CHARGE



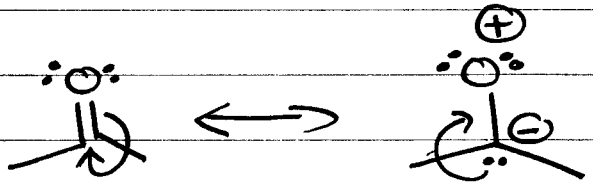
③ π BOND / +VE CHARGE



④ π BOND / TWO EN ATOMS

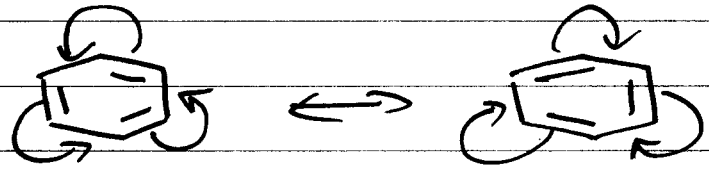


NOT



O is more EN than C

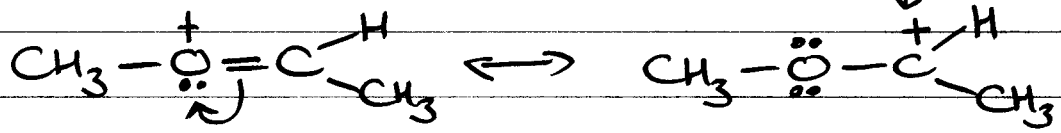
⑤ π BONDS in a RING



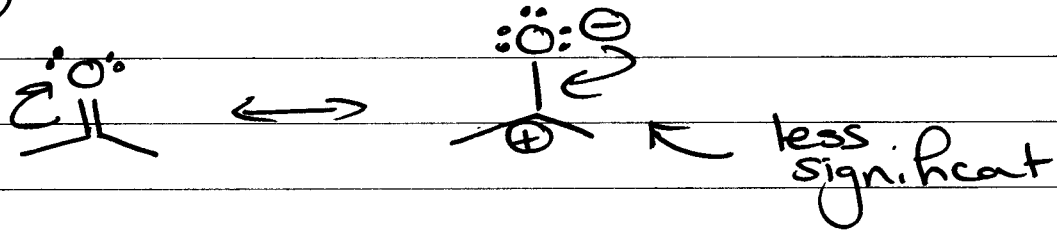
– RELATIVE IMPORTANCE OF CONTRIBUTORS

a) MAXIMISE OCTETS

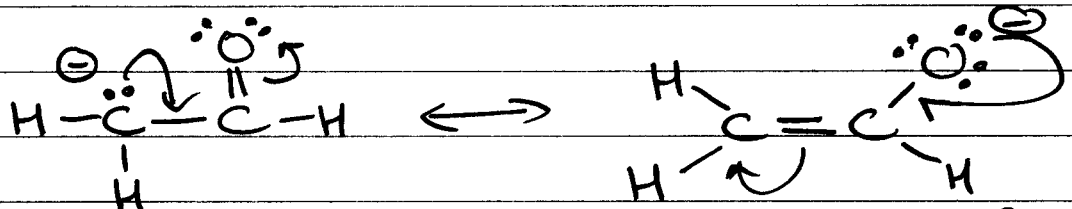
more significant



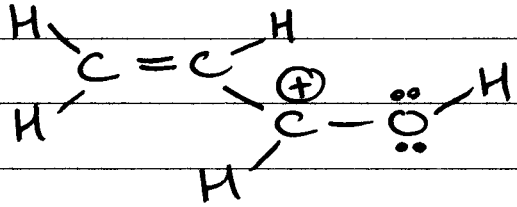
b) MINIMISE CHARGES



c) PUT -VE CHARGE ON MORE EN ELEMENT



HMK



DRAW TWO MORE RESONANCE FORMS

- which is most signi.hcant?
- structure of HYBRID?