LEC (3) CHEM 30A Apr 8th

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

Hmk: READ rest of Ch1
Problems 1.14-1.17, 1.48-1.54 + MOLECULAR STRUCTURES WORKSHEETS

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(1) SHAPES of MOLECULES

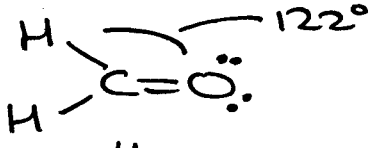
(PAIRS OF ELECTRONS IN VALENCE SHELL)
- BONDED & NONBONDED (lone pairs)

BUT TREAT MULTIPLE BONDS AS SINGLE

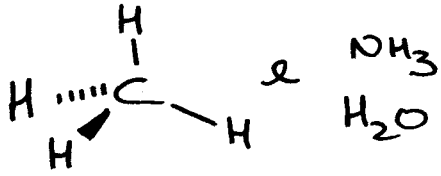
ADD #BP to LP
(or #atoms)

2 → LINEAR

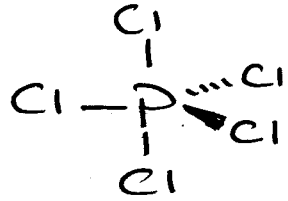
3 → TRIGONAL PLANAR



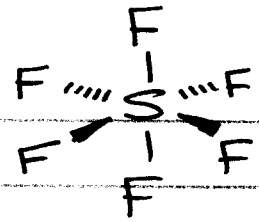
4 → TETRAHEDRAL



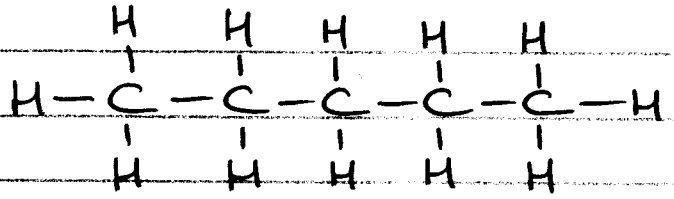
5 → TRIGONAL BIPYRAMIDAL



PCl5

6 → OCTAHEDRAL  SF_6

(2) DRAWING ORGANIC STRUCTURES

a)  ~~PENTANE~~ (structural formula)

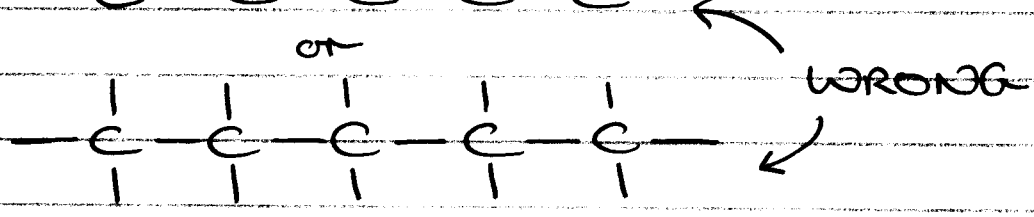
= condensed formula

$CH_3CH_2CH_2CH_2CH_3$ or $CH_3(CH_2)_3CH_3$

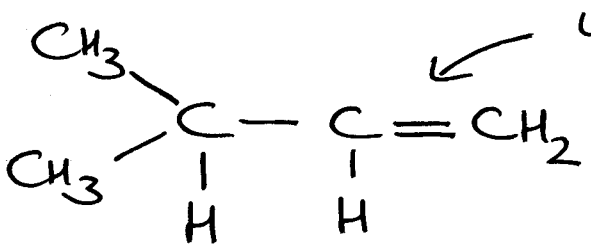
= line formula

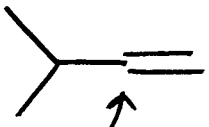
- draw CHAINS as ZIG-ZAGS
- leave out ANY H attached to C
- draw NONBONDED electrons (lone pairs)

DO NOT WRITE

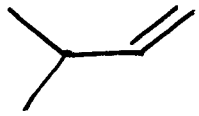


b) $(CH_3)_2CHCHCH_2$?

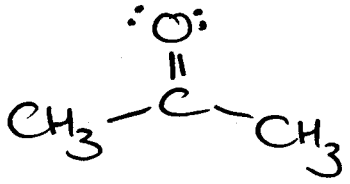


maybe you would draw 

geometry of C atom?
=> TRIGONAL PLANAR

So  TRY to be as true to molecular shape as possible

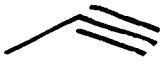
c) $CH_3(CO)CH_3$



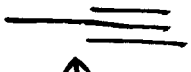
not 

TRIGONAL PLANAR

d) CH_3CCH => $CH_3-C\equiv C-H$

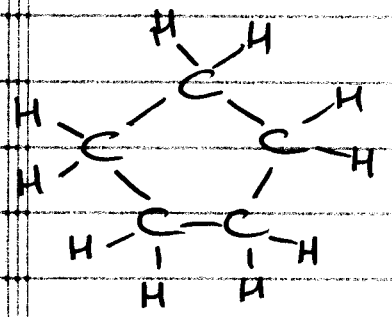
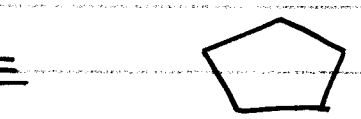


NO!



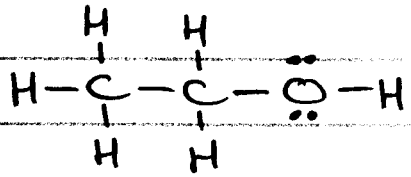
↑
Linear

- RINGS

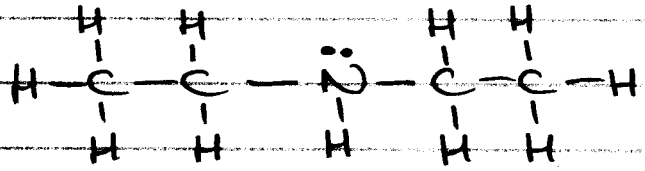



each of these is a CH_2

- HETEROATOMS (draw Hs and lone pairs)




not




not

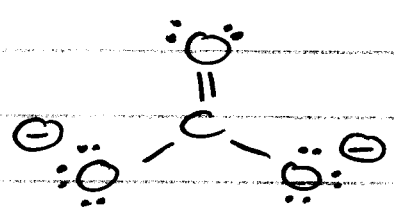
- example C_5H_{12}

CONSTITUTIONAL ISOMERS

- same formula, different arrangements of atoms

(3) RESONANCE

Consider CO_3^{2-}

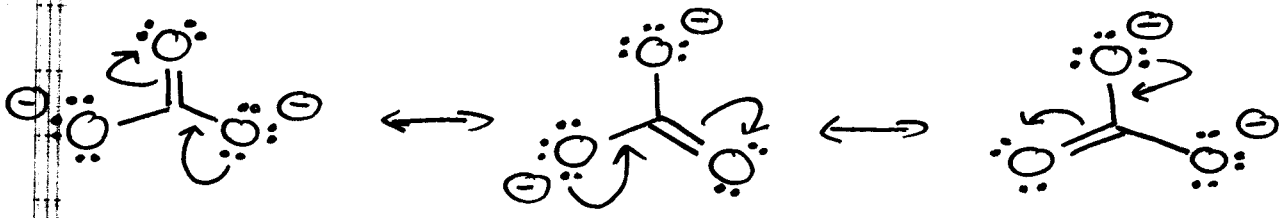


one C=O

two C–O bonds

C=O shorter/stronger bond than C–O

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



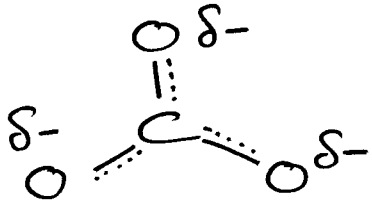
RESONANCE CONTRIBUTORS (ALL EQUIVALENT)

ARROWS ⟷ Separates resonance contributors

↷ CURLY ARROW movement of a pair of electrons

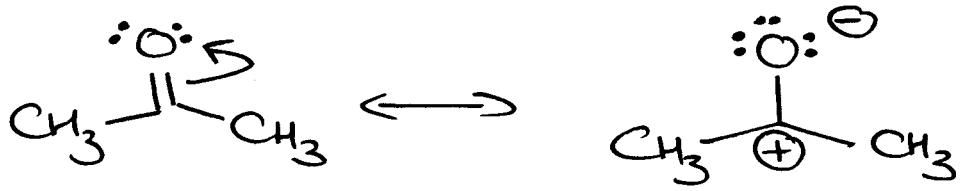
NONE of these contributors actually EXIST!

actual structure is



RESONANCE HYBRID

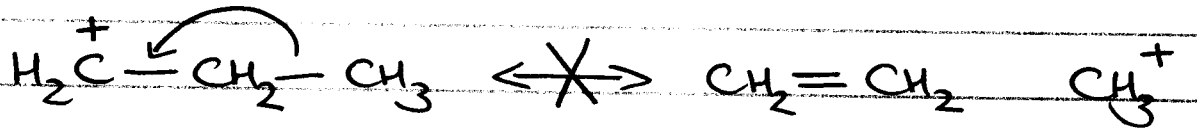
NOT all resonance contributors are necessarily equivalent, for example



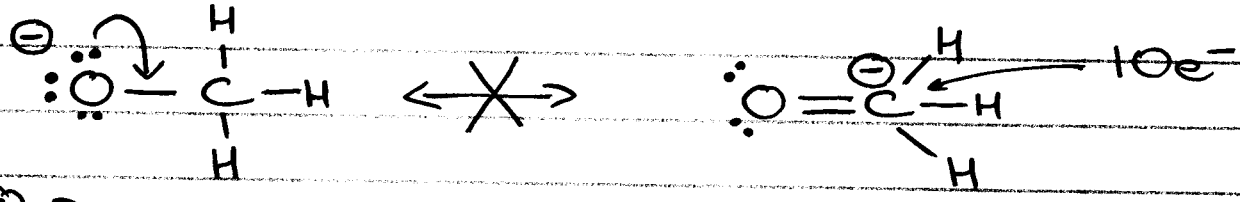
Which one of these is most stable?

- RULES for writing RESONANCE STRUCTURES
- DO NOT

① BREAK ANY SINGLE BONDS



② VIOLATE THE OCTET RULE



③ DO NOT MOVE ATOMS

- DRAWING RESONANCE STRUCTURES

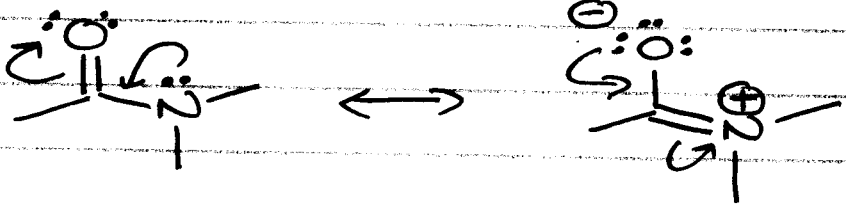
Cannot break single bonds, so we can only move electrons from double (or triple) bonds and lone pairs

PATTERNS

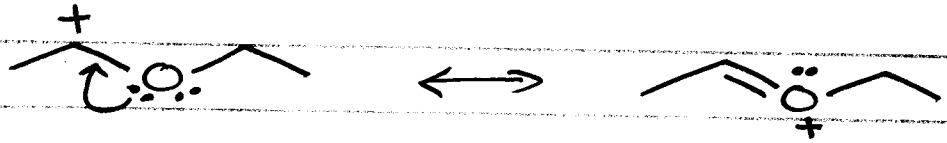
① LONE PAIR NEXT TO π BOND

double or triple bond

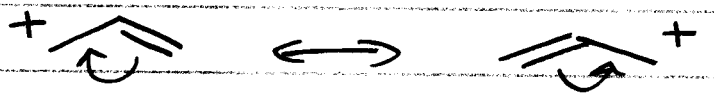
"next to" means one single bond away



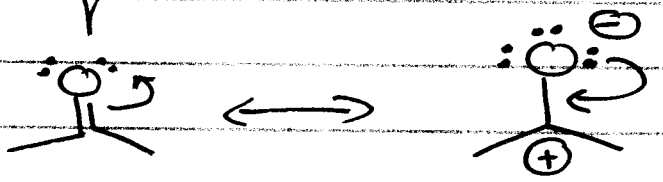
② LONE PAIR NEXT TO +ve CHARGE

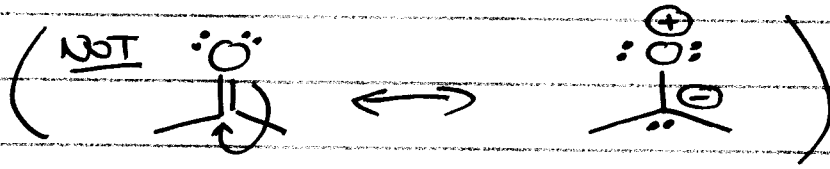


③ π BOND next to +ve CHARGE



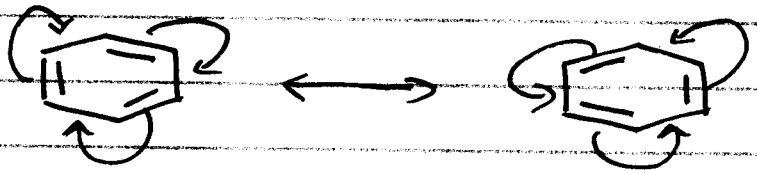
④ π BOND between two atoms where one is quite EN





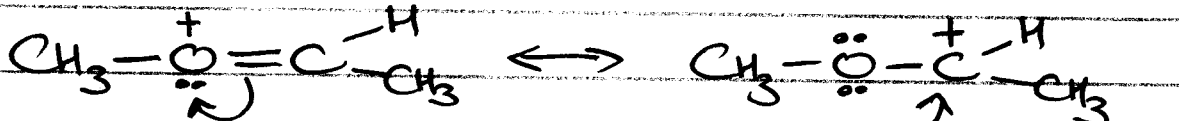
O is more EN than C

⑤ ALTERNATING π BONDS



– RELATIVE IMPORTANCE of CONTRIBUTING STRUCTURES

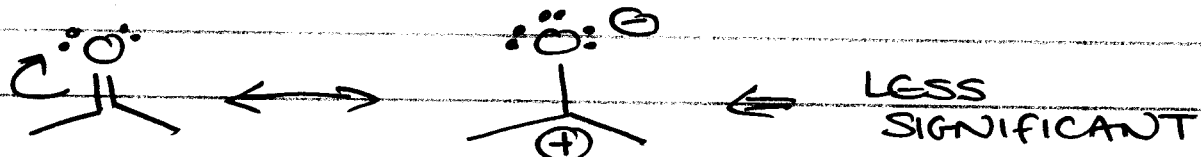
① MAXIMISE OCTETS



more significant

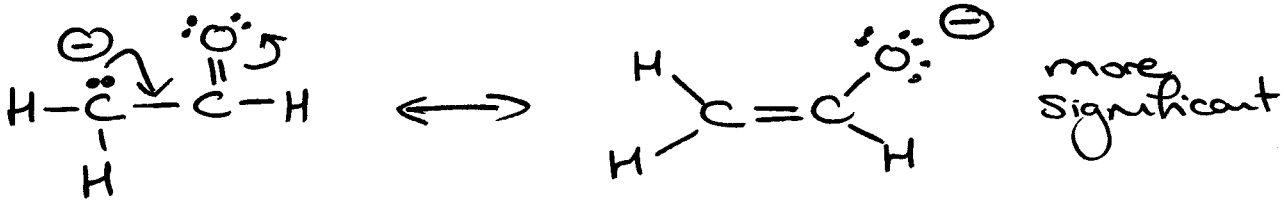
not a full octet

② MINIMISE CHARGES

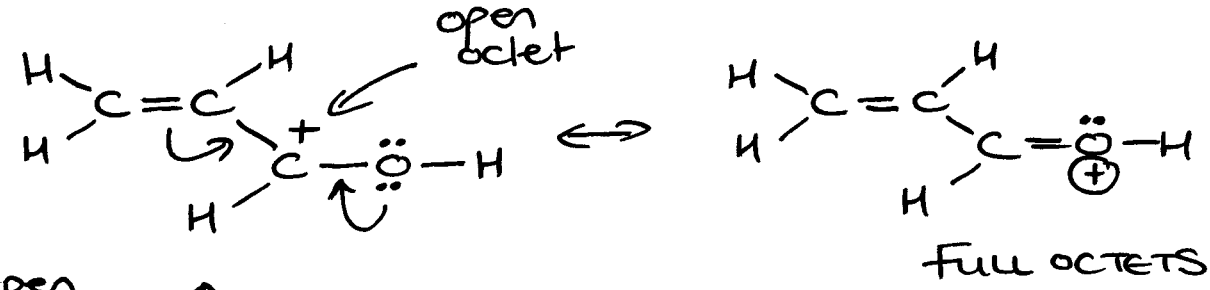


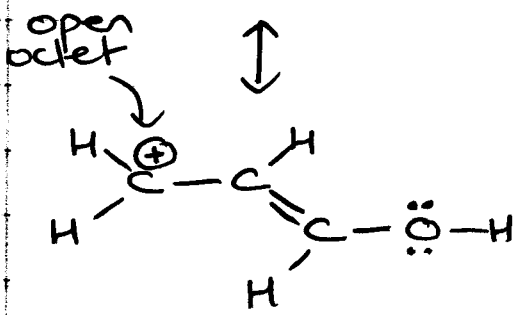
LESS SIGNIFICANT

(3) PUT -ve CHARGE ON MORE EN ELEMENT

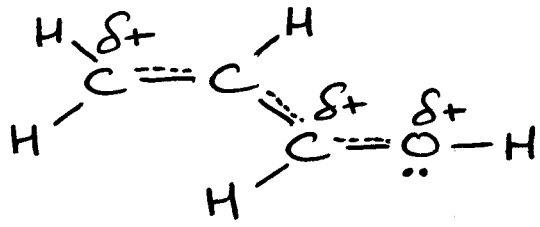


e.g.





HYBRID



next up: ATOMIC ORBITALS