

STRUCTURE AND PROPERTIES OF ORGANIC MOLECULES

WAVE PROPERTIES OF ELECTRONS IN ORBITALS

ELECTRONS HAVE WAVE-LIKE PROPERTIES

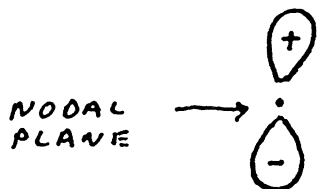
THE 1S ORBITAL IS SPHERICAL

THE WAVE WITHIN IT VIBRATES WITH POSITIVE AND

NEGATIVE AMPLITUDE REPRESENTED WITH + AND - SIGNS

P ORBITALS HAVE 2 LOBES OF ELECTRON DENSITY

WHICH ALWAYS HAVE OPPOSITE SIGNS



MOLECULAR ORBITALS

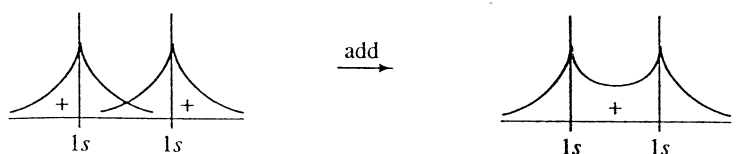
ARE FORMED WHEN TWO ATOMIC ORBITALS OVERLAP

THE RESULTING ORBITAL RESEMBLES A LINEAR COMBINATION OF ATOMIC ORBITALS (LCAO)

IN THESE ORBITALS ELECTRONS VIBRATE IN MORE COMPLEX WAVES

IN THE HYDROGEN MOLECULE 1s ORBITALS OVERLAP TO FORM

A CYLINDRICAL MOLECULAR ORBITAL AND A SIGMA BOND σ



→



bonding molecular orbital

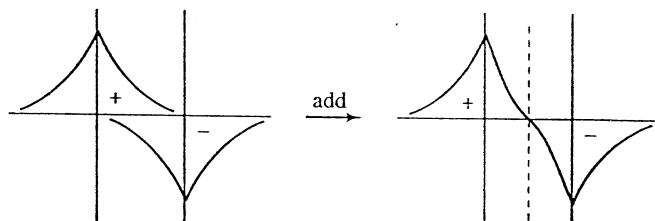
represented by:



→



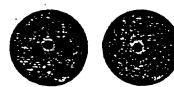
σ -bonding MO



→



antibonding molecular orbital



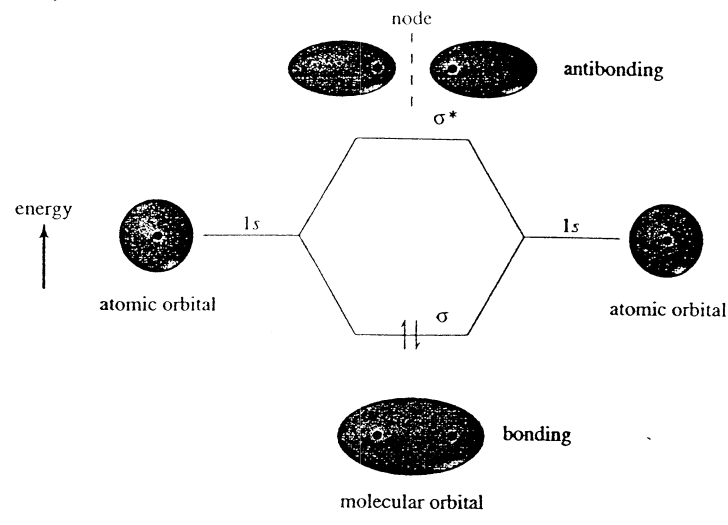
→



σ^* antibonding MO

A HIGHER ENERGY →
ANTI BONDING MOLECULAR
ORBITAL IS ALSO FORMED

THE RELATIVE ENERGY OF 1s ATOMIC AND MOLECULAR ORBITALS



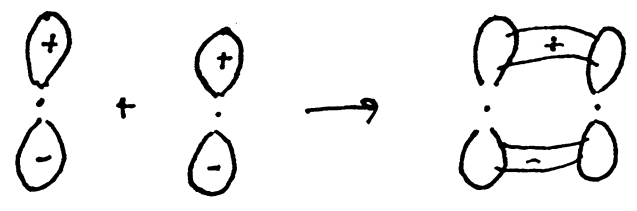
THE OVERLAP OF P ORBITALS ALSO MAKES A σ BOND



AN S AND A P ORBITAL CAN ALSO OVERLAP

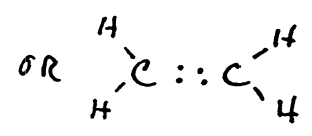
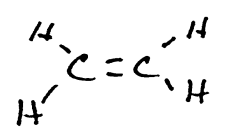


THE SECOND BOND OF A DOUBLE BOND COMES FROM SIDEWAYS OVERLAP OF 2 P ORBITALS



SO A DOUBLE BOND CONSISTS OF A σ BOND PLUS THIS BOND, CALLED A π (PI) BOND

THE DOUBLE BOND



HYBRID ORBITALS

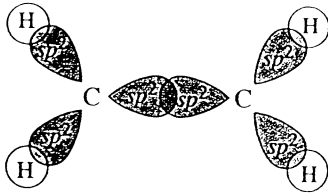
IN ADDITION TO S AND P ORBITALS WE GET A COMBINATION OF BOTH, CALLED HYBRID ORBITALS

FOR EXAMPLE, AN S AND A P ORBITAL MAY INTERACT TO FORM AN sp HYBRID ORBITAL

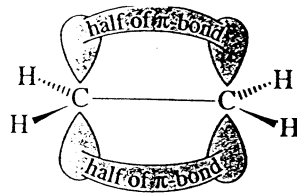
- AN S AND 2 P ORBITALS MAKE $3sp^2$ HYBRIDS
- AN S AND 3 P ORBITALS MAKE $4sp^3$ HYBRIDS

ELECTRON PAIRS IN ELECTRON PAIR BONDS REPEL EACH OTHER
 STABILITY IS GAINED WHEN ELECTRON PAIRS ARE AS FAR APART AS POSSIBLE (VALENCE SHELL ELECTRON PAIR REPELSION) USE VSEPR

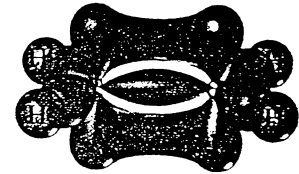
- 2 sp ORBITALS $\rightarrow 180^\circ \rightarrow$ LINEAR GEOMETRY $H-C \equiv C-H$
 3 sp^2 ORBITALS $\rightarrow 120^\circ \rightarrow$ TRIGONAL PLANAR $H_2C=CH_2$
 4 sp^3 ORBITALS $\rightarrow 109.5^\circ \rightarrow$ THE TETRAHEDRAL ANGLE CH_4



σ -bond framework
 (viewed from above the plane)



π bond
 (viewed from alongside the plane)

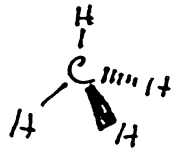


ethylene

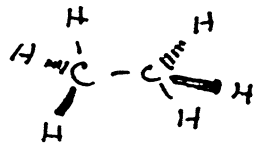
DRAWING MOLECULES IN 3D PERSPECTIVE

DASHED LINES INDICATE BONDS THAT GO AWAY FROM THE READER
 WEDGES INDICATE BONDS THAT COME TOWARDS THE READER

FOR METHANE



FOR ETHANE



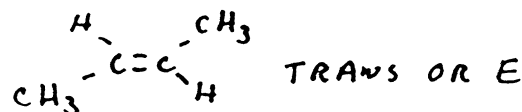
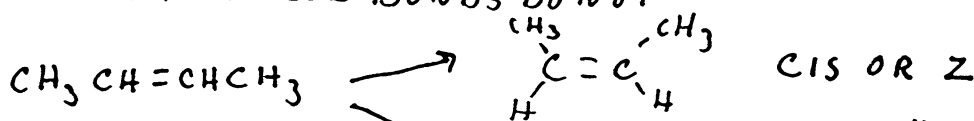
HYBRIDIZATION RULES

- BOTH σ BONDING ELECTRONS RESIDE IN HYBRID ORBITALS
 THE NUMBER OF HYBRID ORBITALS = # OF σ BONDS + # NONBONDING PAIRS
- IN MULTIPLE BONDS
 - FIRST BOND IS A σ
 - 2nd BOND IS A π MADE FROM 2 P ORBITALS
 - 3rd BOND IS A π MADE FROM 2 P ORBITALS

ROTATION AROUND BONDS AND ISOMERISM

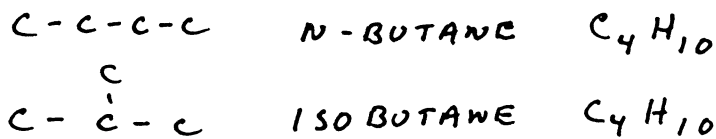
- SINGLE BONDS ALLOW FREE ROTATION

- BUT DOUBLE BONDS DO NOT



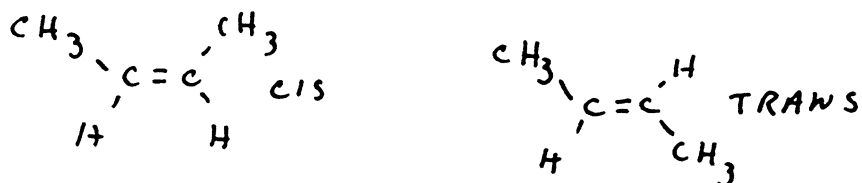
CONSTITUTIONAL ISOMERS, ALSO CALLED STRUCTURAL ISOMERS, HAVE THE SAME NUMBERS AND TYPES OF ATOMS BUT DIFFER IN THEIR BONDING SEQUENCE

FOR EXAMPLE

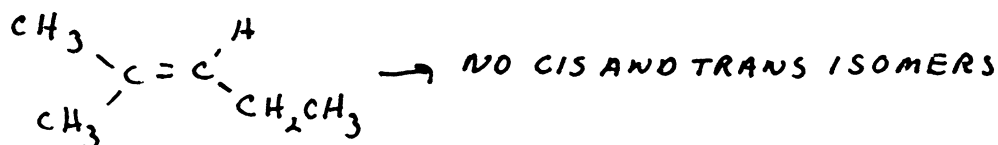


STEREISOMERS

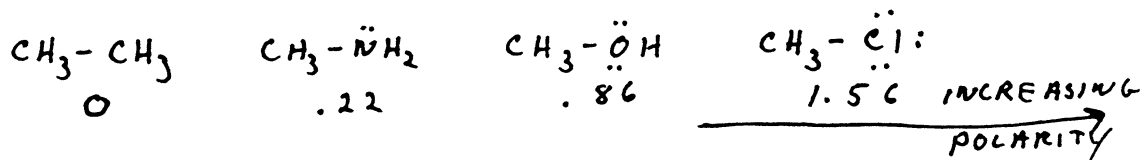
ISOMERS THAT DIFFER ONLY IN SPATIAL ARRANGEMENT AS IN CIS AND TRANS 2-BUTENE



TO HAVE CIS AND TRANS STEREOISOMERS, THERE MUST BE 2 DIFFERENT GROUPS ON EACH END OF THE DOUBLE BOND



MORE ON BOND POLARITY - DIPOLE MOMENTS (D)



THE DIPOLE MOMENT μ IS MEASURED IN DEBYE (D)

$$\mu = \delta \times d = \text{AMOUNT OF CHARGE} \times \text{DISTANCE BETWEEN CHARGES}$$

AS AN APPROXIMATION

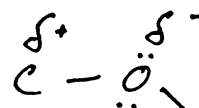
$$\mu = 4.8 \times \delta \times d$$

THIS RELATIONSHIP CAN BE USED TO CALCULATE CHARGE SEPARATION

FOR $\text{C}-\ddot{\text{O}}$ $\mu = 0.86 \text{ D}$
 $d = 1.43 \text{ \AA}$

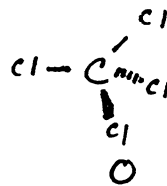
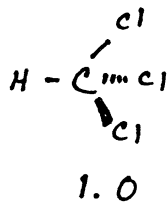
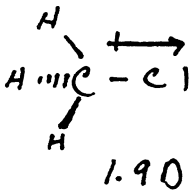
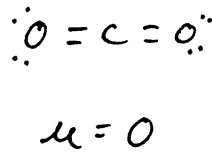
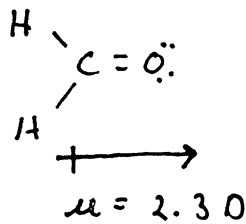
$$0.86 = 4.8 \times 1.43 \times \delta$$

$$\delta = 0.125 \text{ electron CHARGE}$$



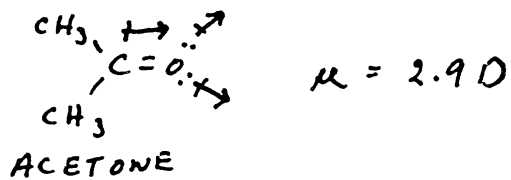
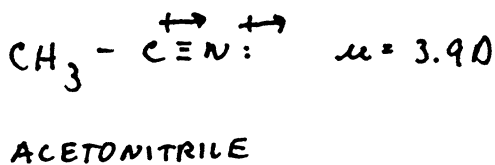
MOLECULAR DIPOLE MOMENTS

EQUAL TO THE VECTOR SUM OF INDIVIDUAL DIPOLE MOMENTS



IN CCl_4 INDIVIDUAL MOMENTS CANCEL

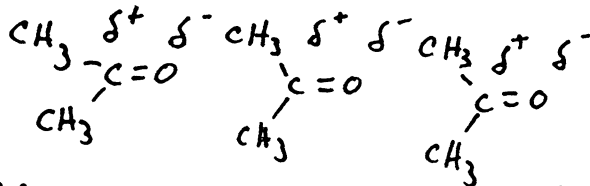
LONE PAIRS HAVE A SIGNIFIGANT EFFECT



INTERMOLECULAR ATTRACTIONS AND REPULSIONS

DIPOLE-DIPOLE

POLAR MOLECULES MOSTLY ALIGN SO THAT THEIR DIPOLES ATTRACT



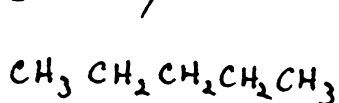
THIS ATTRACTIVE FORCE MUST BE OVERCOME IN MELTING AND BOILING SO A MORE POLAR MOLECULE WILL HAVE A HIGHER BOILING POINT AND MELTING POINT, ALL ELSE BEING EQUAL

THE LONDON DISPERSION FORCE

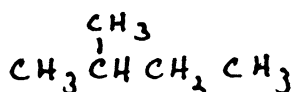
THIS IS THE SMALLEST ATTRACTIVE FORCE

IT RESULTS FROM TEMPORARY, CORRELATED, INDUCED DIPOLES

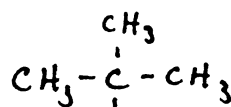
THE LONDON FORCES CAN BE SEEN IN THE BOILING POINTS OF THE VERY NON-POLAR HYDROCARBONS



m-PENTANE BP 36°C



ISOPENTANE BP 28°C



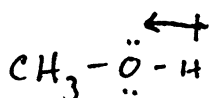
NEOPENTANE BP 10°C

THE MOST HIGHLY BRANCHED ISOMER HAS THE SMALLEST SURFACE AREA OR CONTACT AREA AND THE SMALLEST ATTRACTIVE FORCES

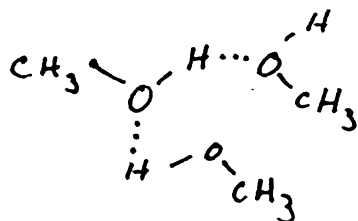
HYDROGEN BONDING

A PARTICULARLY STRONG DIPOLE-DIPOLE ATTRACTION

REQUIRES N-H OR O-H BONDS, WHICH ARE HIGHLY POLAR



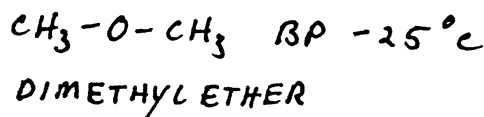
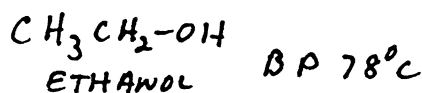
THE HYDROGEN HAS A PARTIAL (+) CHARGE



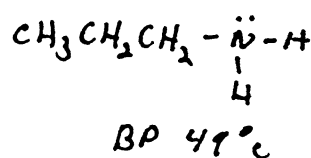
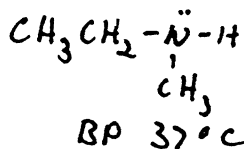
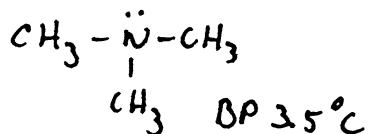
HYDROGEN BONDING

ABOUT 5% AS STRONG AS A C-H BOND

THE DOMINANT INTERMOLECULAR ATTRACTIVE FORCE



IN AMINES



SOLUBILITY "LIKE DISSOLVES LIKE"

POLAR SOLVENTS DISSOLVE POLAR COMPOUNDS

NON POLAR SOLVENTS DISSOLVE NON POLAR COMPOUNDS

OUR TYPICAL POLAR SOLVENT IS WATER

OUR TYPICAL NONPOLAR SOLVENT IS CHLOROFORM, OR CCl₄, OR ALKANES

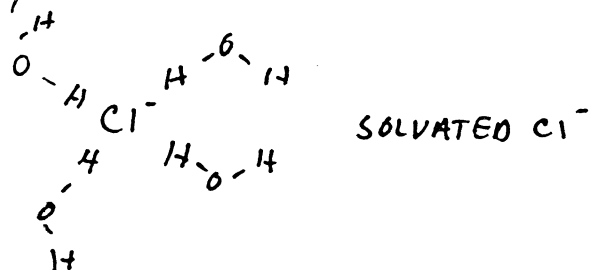
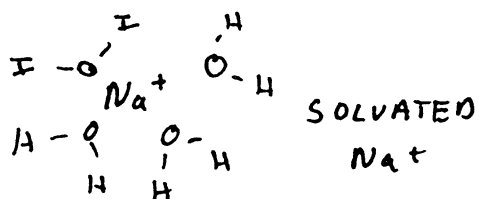
WHEN A COMPOUND DISSOLVES, IT IS SURROUNDED BY SOLVENT MOLECULES OR "SOLVATED"

THIS MAY BE VERY FAVORABLE ENERGETICALLY

SOLVATION

NaCl FORMS A VERY STRONG CRYSTAL LATTICE $MP = 800^{\circ}C$

BUT ADD SALT TO WATER AND IT QUICKLY DISSOLVES



THERE IS QUITE A LARGE RELEASE OF ENERGY UPON SOLVATION

ENTROPY HELPS TOO!

BUT A NON POLAR SOLID, LIKE PARAFFIN WAX $MP \approx 150^{\circ}C$

WILL NOT DISSOLVE IN WATER

THERE IS LITTLE RELEASE IN ENERGY WHEN WAX DISSOLVES, MOSTLY ENTROPY DRIVES DISSOLUTION

THERE IS NOT ENOUGH ENERGY TO DISRUPT THE HYDROGEN BONDS IN H_2O

THERE ARE STRONGER ATTRACTIVE FORCES BETWEEN WAX AND NON POLAR SOLVENTS, SO THATS WHERE WAX DISSOLVES

INTRODUCTION TO THE FUNCTIONAL GROUPS

HYDROCARBONS - COMPOUNDS OF HYDROGEN AND CARBON

ALKANES - ALL SINGLE BONDS

ALKENES - DOUBLE BONDS

ALKYNES - TRIPLE BONDS

AROMATICS - DERIVATIVES OF BENZENE

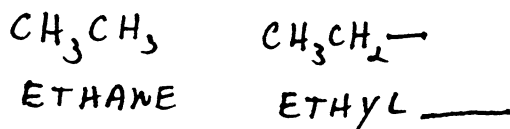
THE PREFIX NUMBERING SYSTEM

NAME	CARBON NUMBER	NAME	CARBON NUMBER
METHANE	1	HEXANE	6
ETHANE	2	HEPTANE	7
PROPANE	3	OCTANE	8
BUTANE	4	NONANE	9
PENTANE	5	DECANE	10

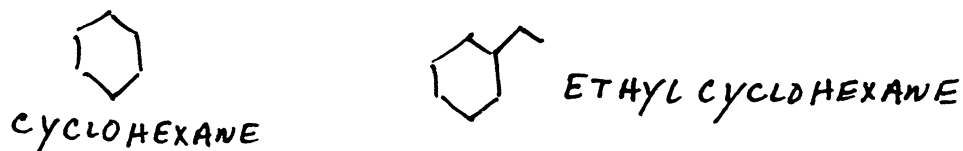
ALKANES

HYDROCARBONS, NAME ENDS IN ANE

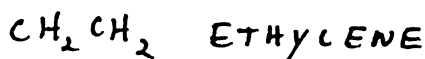
TO NAME A HYDROCARBON PORTION OF A MOLECULE, NAME AS ALKYL GROUP, ENDING IN YL



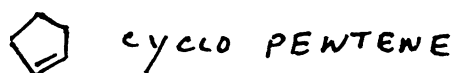
CYCLOALKANES ARE SIMPLY IN A RING



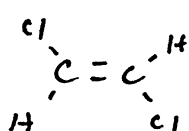
ALKENES FEATURE ONE OR MORE DOUBLE BONDS $\text{C}=\text{C}$
NAMES END IN ENE



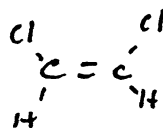
CYCLOALKENES



CIS AND TRANS

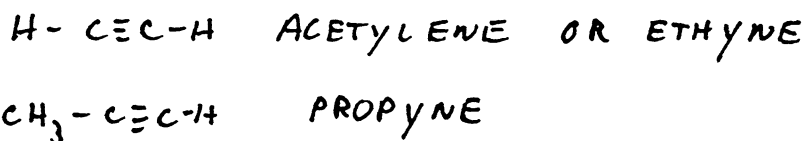


TRANS - 1,2-DICHLOROETHENE



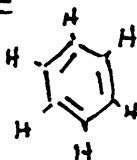
CIS - 1,2-DICHLOROETHENE

ALKYNES - TRIPLE BONDS - END IN YNE

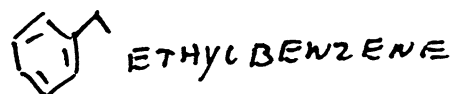


AROMATIC HYDROCARBONS

DERIVATIVES OF BENZENE

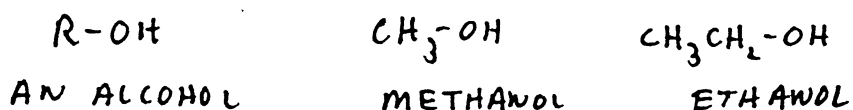


C_6H_6 BENZENE



ORGANIC COMPOUNDS CONTAINING OXYGEN

ALCOHOLS CONTAIN THE HYDROXYL GROUP $-OH$ OL ENDING

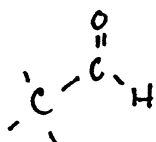


ETHERS CONTAIN THE $C-O-C$ FUNCTIONAL GROUP



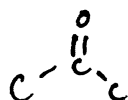
ALDEHYDES AND KETONES CONTAIN THE $\begin{array}{c} O \\ || \\ C \end{array}$ GROUP

ALDEHYDES HAVE 1 CARBON AND 1 HYDROGEN ATTACHED

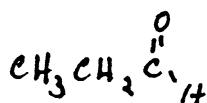


NAMES END IN AL OR ALDEHYDE

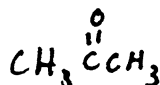
KETONES HAVE 2 CARBONS



NAMES END IN ONE



PROPANAL



PROPANONE

CARBOXYLIC ACIDS

HAVE THE $\begin{array}{c} O \\ || \\ C-OH \end{array}$ GROUP NAMED -OIC ACID



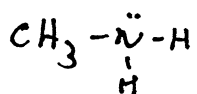
DERIVATIVES OF CARBOXYLIC ACIDS INCLUDE:



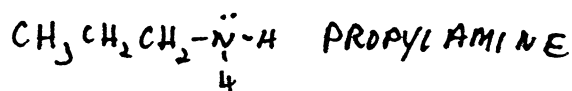
NITROGEN COMPOUNDS INCLUDE

NITRILES $-C \equiv N$

AMINES - DERIVATIVES OF AMMONIA



METHYL AMINE



PROPYL AMINE