20160914

CHM 151:
ORGANIC CHEMISTRY II – III
STRUCTURE & BONDING

OUTLINE:

- ATOMIC STRUCTURE
- LEWIS STRUCTURES & COVALENT BONDING
- VALENCE BOND THEORY
- HYBRID BONDING

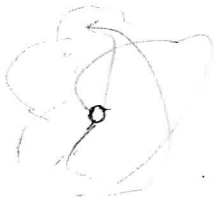
AND MORE

OBJECTIVES

- TO INFER THE CONFIGURATION & NUMBER OF VALENCE ELECTRONS
- DRAW A LEWIS DOT STRUCTURE
- PREDICT THE HYBRIDIZATION STATE AND NUMBER OF LONE PAIRS.

AND MORE.

ATOMIC STRUCTURE



Z: NO. OF PROTONS IN THE NUCLEUS

A: NO OF PROTONS + NO. OF NEUTRONS

ISOTOPES:

$Z_1 = Z_2$, $A_1 \neq A_2$

ORBITALS

s p d

- **AUFBAU PRINCIPLE**: THE LOWEST-ENERGY ORBITALS ARE FILLED FIRST

- **PAULI EXCLUSION PRINCIPLE**: ORBITALS ACCOMODATE A MAXIMUM OF TWO ELECTRONS, HAVING OPPOSITE SPINS

  NOTATION FOR SPINS: $1\downarrow$

- **HUND'S RULE**: IF MULTIPLE ORBITALS OF EQUAL ENERGY ARE AVAILABLE, FILL THEM INDIVIDUALLY WITH PARALLEL SPINS FIRST

eg

	p_x	p_y	p_z
1.	1		
2.	1	1	
3.	1	1	1
4.	$1\downarrow$	1	1

ELECTRONIC CONFIGURATIONS

	Z		
H	1	1 s	↑
C	6	2 p	↑ ↑
		2 s	↑↓
		1 s	↑↓
P	15	3 p	↑ ↑ ↑
		3 s	↑↓
		2 p	↑↓ ↑↓ ↑↓
		2 s	↑↓
		1 s	↑↓
S	16	3 p	↑↓ ↑ ↑
		3 s	↑↓
		2 p	↑↓ ↑↓ ↑↓
		2 s	↑↓
		1 s	↑↓
Br	35	4 p	↑↓ ↑↓ ↑
		3 d	↑↓ ↑↓ ↑↓ ↑↓ ↑↓
		4 s	↑↓
		3 p	↑↓ ↑↓ ↑↓
		3 s	↑↓
		2 p	↑↓ ↑↓ ↑↓
		2 s	↑↓
		1 s	↑↓

VALENCE ELECTRONS

CHEMICAL BONDING

WHY DO ATOMS FORM BONDS?

IT IS THERMODYNAMICALLY FAVOURABLE TO FORM A BOND.

? GIBB'S FREE ENERGY

OCTET RULE:

IN MOST CASES, THE BOND FORMATION CONVERGES TO SUCH A STATE THAT THE RESULTANT CONFIGURATION IS SIMILAR TO A NOBLE GAS CONFIGURATION.

- COVALENT vs IONIC BONDING — THE DIFFERENCE IN ELECTRONEGATIVITY DETERMINCE THE DIFFERENCE IN THE BONDS.

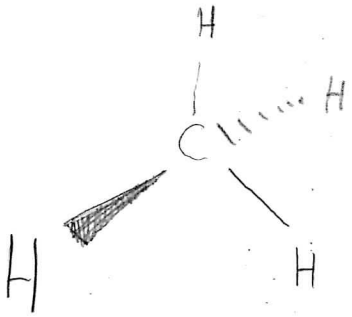
COVALENT BONDING

:.:. VALENCE ELECTRONS ARE REPRESENTED BY DOTS.

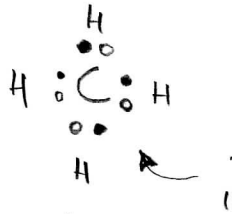
ALT:
LINE-BOND REPRESENTATION
SHOWS COVALENT BONDS
AS LINES BETWEEN
THE ATOMS

EXAMPLE

METHANE



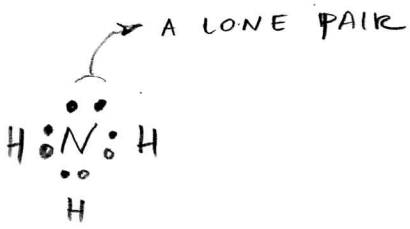
Kekulé



THE ELECTRONS IN THE BOND ARE EQUIVALENT

LEWIS

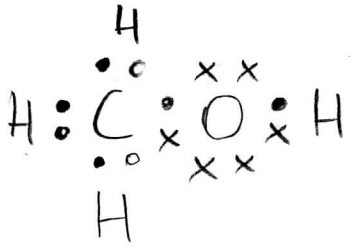
AMMONIA

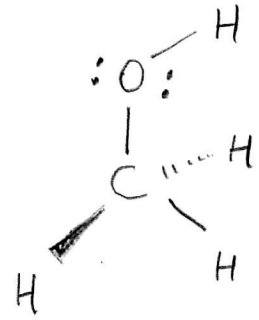


LEWIS

KEKULÉ

METHANOL





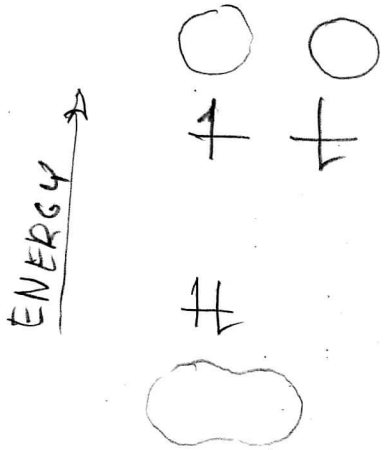
VALENCE BOND THEORY

:: COVALENT BONDS RESULT FROM THE OVERLAP OF SINGLY BOUND ORBITALS OF THE ATOMS INVOLVED.

BOND CHARACTERIZATION: • STRENGTH [kJ/mol] / [kcal/mol]

• LENGTH [pm] / [Å]

2 HYDROGEN ATOMS



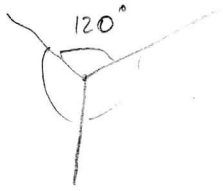
HYDROGEN MOLECULE

VALENCE BOND THEORY

MOLECULES WITH MULTIPLE COVALENT BONDS ARE DESCRIBED BY INVOKING HYBRID ORBITALS.

HYBRID ORBITALS FORM FROM LINEAR COMBINATION OF SINGLE ORBITALS.

EXAMPLE



TETRAHEDRAL

sp^3