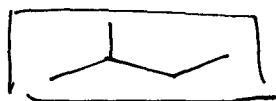


Lecture Notes From 9/16/02

→ new homework problems available today

Review: nomenclature



- ① designate parent chain : butane
- ② determine appendage name : methyl
- ③ indicate appendage position on chain : 2

name: 2-methylbutane

→ all problems from homework #1 can now be answered based on what we have learned in lecture.

TODAY

- ① Atomic Orbitals
- ② Molecular Orbitals

▶ Quantum Mechanics

- This is the basis for orbital theory
- a good overview from a non-scientific type book can be found in "The making of the Atomic Bomb" by R. Rhodes

▶ Schrodinger Equation

- An equation derived to describe a negatively charged e^- in the vicinity of ~~an~~ a nucleus. The solution is represented by the symbol ψ and is called a wave function

$$\boxed{-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + U(x)\psi(x) = E\psi(x)}$$

* you don't need to know this eq'n *

ψ^2 = probability of a given e^- density at a given point in space

note:
A good explanation of this material can be found in Organic Chemistry by M. Jones ch 1-4.

• Each wave function can be described by a set of quantum numbers:

- $n \propto$ distance from nucleus
- $l \propto$ shape of orbital
- $m_l \propto$ orientation.
- $s \propto$ spin (1/2)

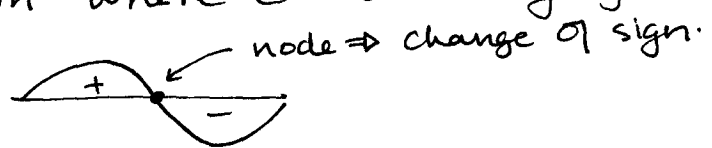
Energy	n	l	m_l	s	orbital
low	1	0	0	$\pm 1/2$	1s
↓	2	0	0	$\pm 1/2$	2s
high	2	1	-1, 0, +1	$\pm 1/2$	2p

↑ (x, y, z axis)

► Consider 1s Orbital

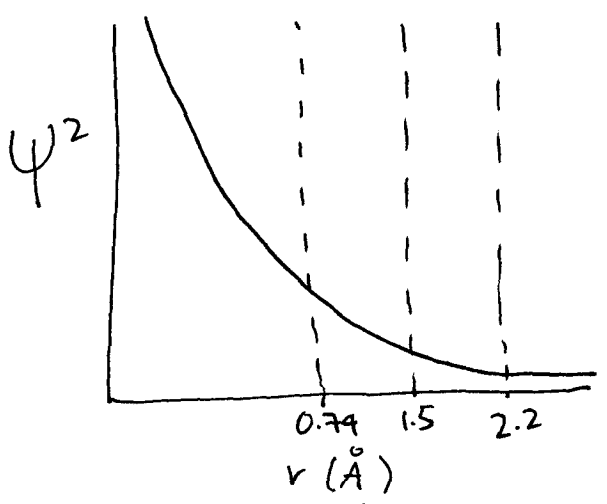
- $n = 1$, ∴ no nodes (# nodes = $n - 1$)
- $l = 0$, ∴ symmetrically spherical

node: position where e^- density goes to zero



this makes sense when atom behavior is described as a wave not a particle.

Probability of e^- density: ψ^2



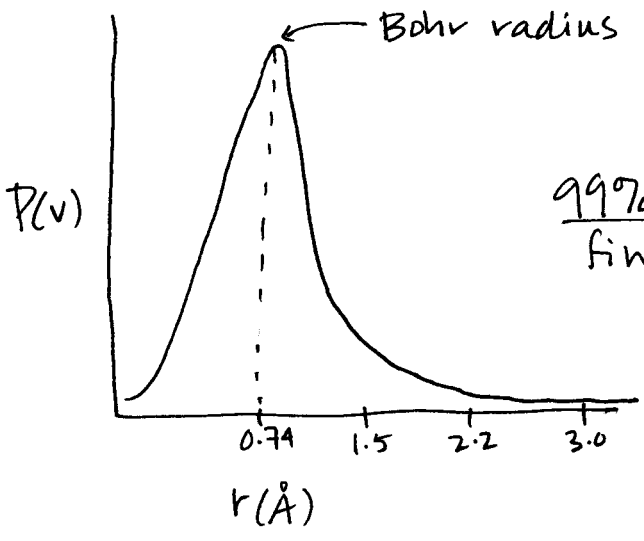
90% of e^- density is at 1.5 Å or less.

note

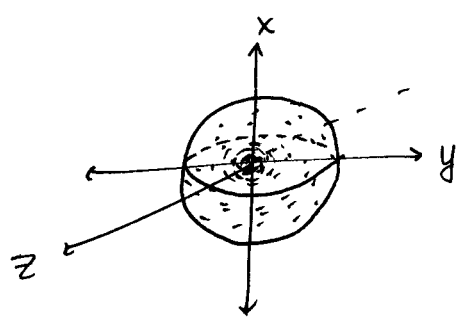
this probability has nothing to do with the # of e^- in a given space. This graph describes 1s which has 2 e^- only

↑ distance from nucleus

Probability of Finding an e^- at a given position in $1s : P(r)$



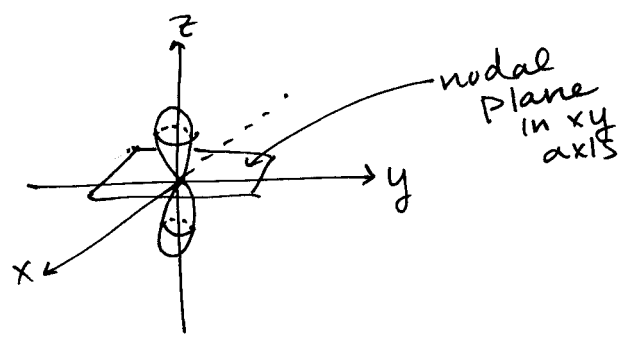
99% probability of finding e^- at $\leq 2.2 \text{ \AA}$



To understand the probability of a given position, you must consider the volume the e^- density exists in. That is what the above graph does ($P(r)$)

Consider $2p$ Orbital

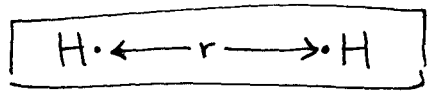
- $n = 2, \therefore 1 \text{ node}$
- $l = 1, \therefore \text{dumbbell shaped}$



maximal e^- density along z-axis

Molecular Orbitals

→ consider H_2



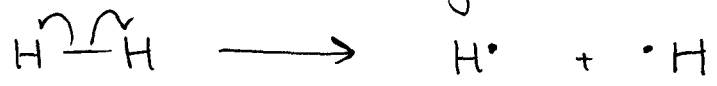
how does energy change as you vary r ?

→ we know certain things:

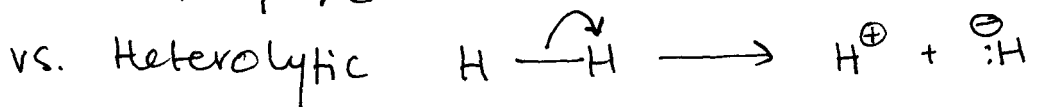
① Bond Dissociation Energy = +104 kcal/mol (ΔH)

∴ endothermic

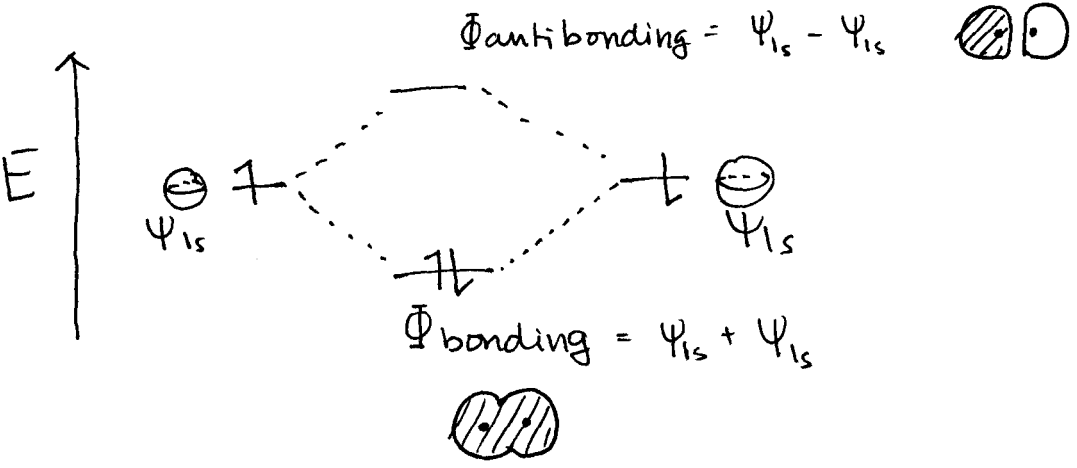
- It describes a homolytic bond cleavage where one electron goes w/ each H.



we use \curvearrowright (half headed arrows) to describe the movement of 1e⁻

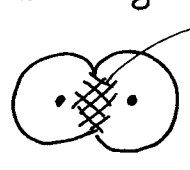


Orbital Interaction Diagrams



▶ molecular orbitals are a linear combination of atomic orbitals.

Bonding:



the e^- density is maximized between the nuclei stabilizing the diatomic molecule and hence lowering the energy

→ This a very compelling argument as to why H is diatomic!

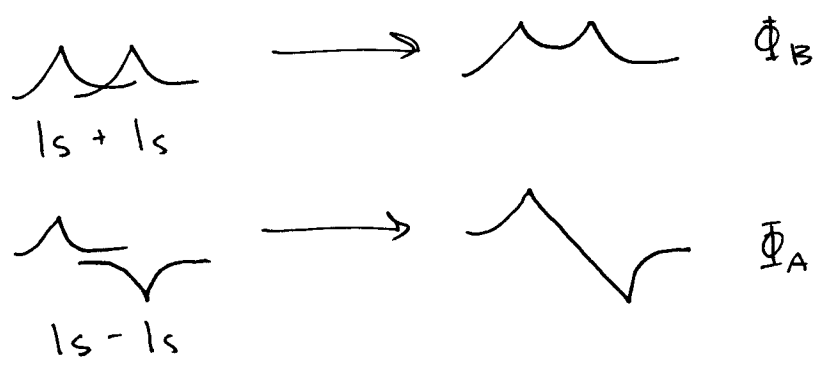
Antibonding:



shading indicates that the orbitals have opposite signs (+/-) These have equal e^- density in each side.

Analogy:

constructive & destructive interference of waves

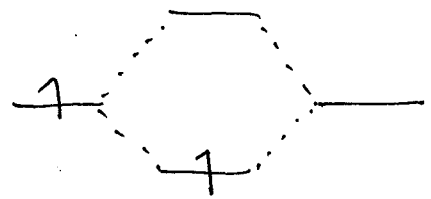


Note:

when writing MO diagrams:

- ① #AO = #MO
- ② $E_{MO} \uparrow$ as # nodes \uparrow
- ③ AOs close in energy interact strongly
- ④ relative shapes of AOs influence interactions

What about H_2^+

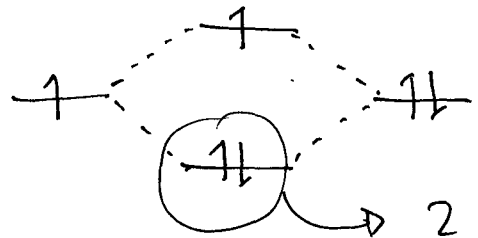


Where is the e^- ?

→ Always in lower energy orbitals which is lower MO or AO?

→ MO - so molecule is still diatomic

What about H_2^0



2 e^- still reside in a low energy molecule. This is more stable as a diatomic molecule than as 2 atoms.