new homework problems available today

Review: nomenclature

- designate parent chain: butane
- determine appendage name: methyl
- 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

\[-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + U(x)\Psi(x) = E\Psi(x)\]

\(\Psi^2\) = 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:

- \( n \) = distance from nucleus
- \( l \) = shape of orbital
- \( m_e \) = orientation
- \( s \) = spin (\( \uparrow \) or \( \downarrow \))

<table>
<thead>
<tr>
<th>Energy</th>
<th>( n )</th>
<th>( l )</th>
<th>( m_e )</th>
<th>( s )</th>
<th>Orbital</th>
</tr>
</thead>
<tbody>
<tr>
<td>low</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>( \pm \frac{1}{2} )</td>
<td>1s</td>
</tr>
<tr>
<td>high</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>( \pm \frac{1}{2} )</td>
<td>2s</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1</td>
<td>-1, 0, +1</td>
<td>( \pm \frac{1}{2} )</td>
<td>2p</td>
</tr>
</tbody>
</table>

Consider 1s Orbital:

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

Node: position where \( \psi \) density goes to zero

Node \( \Rightarrow \) change of sign.

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

Probability of \( \psi \) density: \( \psi^2 \)

90% of \( \psi \) density is at 1.5 Å or less.

*Note*

This probability has nothing to do with the \# of \( \psi \) in a given space. This graph describes 1s which has 2\( \psi \) only.
Probability of finding an $e^\theta$ at a given position in $1s : P(r)$

99.7% probability of finding $e^\theta$ at $\leq 2.2\,\text{Å}$

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

Consider $2p$ Orbital

$n = 2, \quad \therefore 1\,\text{node}$

$l = 1, \quad \therefore \text{dumbbell shaped}$

maximal $e^\theta$ density along $z$-axis
Molecular Orbitals

→ consider $H_2$

\[ H \leftarrow r \rightarrow H \]

how does energy change as you vary $r$?

→ we know certain things:

0. Bond Dissociation Energy = $+104$ kcal/mol ($\Delta H$)
   .: endothermic

• It describes a homolytic bond cleavage where one electron goes with each $H$.

\[ H \underset{r}{\overset{r}{\rightarrow}} H^+ + \cdot H \]

\[ \text{we use } \sim (\text{half-headed arrows}) \text{ to describe} \]

the movement of 1 e\(^{-}\)

vs. Heterolytic \[ H \overset{r}{\underset{r}{\rightarrow}} H^+ + \cdot H \]


Orbital Interaction Diagrams

\[ \Phi_{\text{antibonding}} = \Psi_{1s} - \Psi_{1s} \]

\[ \Phi_{\text{bonding}} = \Psi_{1s} + \Psi_{1s} \]

→ molecular orbitals are a linear combination

of atomic orbitals.
Bonding:

- The $e^0$ density is maximized between the nuclei stabilizing the diatomic molecule and hence lowering the energy.

- This is a very compelling argument as to why H is diatomic.

Antibonding:

- Shading indicates that the orbitals have opposite signs (+/-).
- These have equal $e^0$ density in each side.

Analogy:

- Constructive vs. destructive interference of waves.

\[ \begin{align*}
1s + 1s &\rightarrow \Phi_B \\
1s - 1s &\rightarrow \Phi_A
\end{align*} \]

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 $\text{H}_2^+$

- Where is the $e^-$?
  - Always in lower energy orbitals

- Which is lower MO or AO?
  - MO-so molecule is still diatomic

What about $\text{H}_2^-$

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