Welcome to 3.091

Lecture 10
September 30, 2009

Hybridized & Molecular Orbitals; Paramagnetism
3.091 Test #1
Wednesday, October 7, 2009
Room Assignments

A – Ha: 10-250
He - Sm: 26-100
So - ∞: 4-270
Increasing Electronegativity, $\chi$

- **s Block**
- **p Block**
- **d Block**
- **f Block**

Image by MIT OpenCourseWare.
\[
\% \text{ ionic character} = \left\{ 1 - \exp\left( -\frac{1}{4} (\Delta X)^2 \right) \right\} \times 100
\]

### % Ionic Character of a Single Chemical Bond

<table>
<thead>
<tr>
<th>Difference in Electronegativity</th>
<th>%IC (by L. Pauling)</th>
<th>%IC (by Hannay &amp; Smyth)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.2</td>
<td>1.6</td>
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<tr>
<td>0.2</td>
<td>1.0</td>
<td>3.3</td>
</tr>
<tr>
<td>0.3</td>
<td>2.2</td>
<td>5.1</td>
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<tr>
<td>0.4</td>
<td>3.9</td>
<td>7.0</td>
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<tr>
<td>0.5</td>
<td>6.1</td>
<td>8.9</td>
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<tr>
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<td>8.6</td>
<td>11.0</td>
</tr>
<tr>
<td>0.7</td>
<td>12.0</td>
<td>13.0</td>
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<tr>
<td>0.8</td>
<td>15.0</td>
<td>15.0</td>
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<tr>
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<td>17.0</td>
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<tr>
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<td>22.0</td>
<td>20.0</td>
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<tr>
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<td>27.0</td>
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<tr>
<td>1.4</td>
<td>39.0</td>
<td>29.0</td>
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<tr>
<td>1.5</td>
<td>43.0</td>
<td>32.0</td>
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<tr>
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<td>35.0</td>
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<tr>
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<td>37.0</td>
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<tr>
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<td>56.0</td>
<td>40.0</td>
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<tr>
<td>3.2</td>
<td>92.0</td>
<td>87.0</td>
</tr>
</tbody>
</table>
Group Classifications

Atomic Number

Oxidation States

Symbol

Electronic Configuration

Name

Atomic Weight

Melting Point

Boiling Point

Density

Electronegativity

First Ionization Potential
Electron-Pair Bond

H

1

1s

H

1

1s

H₂
Molecular Orbital ——— Bonding
Molecular Orbital ———— Antibonding
<table>
<thead>
<tr>
<th></th>
<th>He (AO)</th>
<th>He$_2^+$ (MOs)</th>
<th>He$^+$ (AO)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>E</strong></td>
<td><img src="image" alt="Diagram" /></td>
<td><strong>$\sigma_{1s}^*$</strong></td>
<td><strong>$\sigma_{1s}$</strong></td>
</tr>
<tr>
<td><img src="image" alt="E" /></td>
<td><img src="image" alt="Diagram" /></td>
<td><img src="image" alt="Diagram" /></td>
<td><img src="image" alt="Diagram" /></td>
</tr>
</tbody>
</table>

*Image by MIT OpenCourseWare.*
$2p_{za}$ and $2p_{zb}$ combine to form $\sigma_{2p}^*$ antibonding and $\sigma_{2p}$ bonding orbitals.
Bonding

Atomic orbitals

Molecular orbital

Image by MIT OpenCourseWare.
\( \pi_{2p_x}^* \) Antibonding

\( \pi_{2p_x} \) Bonding
Bonding

**Atomic orbitals**

1. $np_x$ + $np_x$
2. $np_y$ + $np_y$

**Molecular orbitals**

1. $\pi np_x$
2. $\pi np_y$
e.g. N$_2$, B$_2$, C$_2$
\[ \text{N}_2 \]

6 bonding electrons

\[ \Rightarrow \text{triple bond} \]

\[ \text{N} \equiv \text{N} \]

946 kJ/mol

Image by MIT OpenCourseWare.
e.g. $O_2$ & $F_2$
\( \sigma_{2p}^* \)  
\( \pi_x^* \)  \( \pi_y^* \)  
\( \sigma_{2p} \)  
\( \pi_x \)  \( \pi_y \)
$\text{O}_2$

6 bonding electrons
2 anti bonding electrons
$\Rightarrow$ double bond

$0 = 0$

498 kJ/mol
$F_2$  
6 bonding electrons  
4 anti bonding electrons  
$\Rightarrow$ single bond  
$F-F$  
160 kJ/mol
Paramagnetism

(a) No magnetic field

(b) Magnetic field turned on

Unpaired electrons
paramagnetism in liquid oxygen

O₂

6 bonding electrons
2 anti bonding electrons
⇒ double bond

= 0
498 kJ/mol

Image by MIT OpenCourseWare.

Three sp² Hybrid Orbitals

An sp² Hybrid Orbital

Hybridization

An sp²-Hybridized Atom

Image by MIT OpenCourseWare.
(a) $\text{C}_2\text{H}_4$ sigma-bonded framework

(b) $\text{C}_2\text{H}_4$ pi bonding

Image by MIT OpenCourseWare.
Extremes in electronegativity

NaI: $\Delta \chi = 1.73$
CsAu: $\Delta \chi = 1.75$

Cs and Au, both metals, melt to form metallic liquids, *but*…
when the concentration nears 50%
(equal numbers of donors & acceptors)

$\bullet^*$ electron transfer occurs $\bullet^*$ !

\[
\text{Cs} \rightarrow \text{Cs}^+ + e^-
\]

\[
\text{Au} + e \rightarrow \text{Au}^-
\]
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metallic melt turns into molten salt!!

- 🌟 clear, colorless liquid
- ⛔️ big drop in electrical conductivity
- 🚀 shift from electronic to ionic conduction
Specific electrical conductivity of liquid Cs–Au alloys as a function of concentration (Hoshino et al. 1975)

![Graph showing the electrical conductivity of Cs–Au alloys at 600°C](Image by MIT OpenCourseWare)
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- cesium auride

Abrerg!
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