Chapter 9
Molecular Geometries and Bonding Theories
Molecular Shapes

- we’ve learned to draw Lewis structures and account for all the valence electrons in a molecule.
- But: Lewis structures are two dimensional and molecules are 3 dimensional objects.
- The 3D structure is absolutely critical for understanding molecules.
Molecular Shapes

- geometry & shape of molecule critical
- we can easily predict the 3D structure of a molecule just by adding up:
  - bound atoms + lone pairs
What Determines the Shape of a Molecule?

- atoms and lone pairs take up space and prefer to be as far from each other as possible
- shape can be predicted from simple geometry
“Things”

- The central atom has four “things” around it. A “thing” is an atom or a lone pair of electrons.

- \# things = atoms plus lone pairs
Valence Shell Electron Pair Repulsion Theory (VSEPR)

“The best arrangement of a given number of things is the one that minimizes the repulsions among them.”
### Geometries

These are the geometries for two through six things around a central atom.

<table>
<thead>
<tr>
<th>number of things</th>
<th>arrangement</th>
<th>geometry</th>
<th>bond angles</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td></td>
<td>Linear</td>
<td>180°</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>Trigonal planar</td>
<td>120°</td>
</tr>
<tr>
<td>4</td>
<td></td>
<td>Tetrahedral</td>
<td>109.5°</td>
</tr>
<tr>
<td>5</td>
<td></td>
<td>Trigonal bipyramidal</td>
<td>120°, 90°</td>
</tr>
<tr>
<td>6</td>
<td></td>
<td>Octahedral</td>
<td>90°</td>
</tr>
</tbody>
</table>
All one must do is count the number of “things” in the Lewis structure.

The geometry will be that which corresponds to that number of “things.”
Molecular Geometries

- The geometry is often \textit{not} the shape of the molecule, however.
- The \textit{shape} is defined by the positions of \textit{only} the atoms in the molecules, not the lone pairs.
Geometries vs. shape

Within each geometry, there might be more than one shape.
Linear geometry

two things

- In this geometry, there is only one molecular geometry: linear.
- NOTE: If there are only two atoms in the molecule, the molecule will be linear no matter what the geometry is.
There are two molecular geometries:

- Trigonal planar, if there are no lone pairs
- Bent, if there is a lone pair.
Lone pairs and Bond Angle

• Lone pairs are physically larger than atoms.
• Therefore, their repulsions are greater; this tends to decrease bond angles in a molecule.
Multiple Bonds and Bond Angles

- Double and triple bonds place greater electron density on one side of the central atom than do single bonds.
- Therefore, they also affect bond angles.
There are three molecular geometries:
- Tetrahedral, if no lone pairs
- Trigonal pyramidal if one is a nonbonding pair
- Bent if there are two nonbonding pairs

<table>
<thead>
<tr>
<th>Things</th>
<th>geometry</th>
<th>atoms</th>
<th>lone pairs</th>
<th>shape</th>
<th>example</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>Tetrahedral</td>
<td>4</td>
<td>0</td>
<td></td>
<td>H(\cdot)H</td>
</tr>
<tr>
<td>3</td>
<td>Trigonal pyramidal</td>
<td>1</td>
<td>1</td>
<td></td>
<td>(\cdot)N(\cdot)H</td>
</tr>
<tr>
<td>2</td>
<td>Bent</td>
<td>2</td>
<td>2</td>
<td></td>
<td>(\cdot)H(\cdot)O</td>
</tr>
</tbody>
</table>
Trigonal Bipyramidal geometry
5 things

- There are two distinct positions in this geometry:
  - Axial
  - Equatorial
Trigonal Bipyramidal geometry

Lower-energy conformations result from having lone pairs in equatorial, rather than axial, positions in this geometry.
There are four distinct molecular geometries in this domain:
- Trigonal bipyramidal
- Seesaw
- T-shaped
- Linear
All positions are equivalent in the octahedral domain.
There are three molecular geometries:

<table>
<thead>
<tr>
<th>Things</th>
<th>geometry</th>
<th>atoms</th>
<th>lone pairs</th>
<th>shape</th>
<th>example</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>Octahedral</td>
<td>6</td>
<td>0</td>
<td>Octahedral</td>
<td>SF$_6$</td>
</tr>
<tr>
<td>5</td>
<td></td>
<td>1</td>
<td></td>
<td>Square pyramidal</td>
<td>BrF$_5$</td>
</tr>
<tr>
<td>4</td>
<td></td>
<td>2</td>
<td></td>
<td>Square planar</td>
<td>XeF$_4$</td>
</tr>
</tbody>
</table>
Larger Molecules

In larger molecules, we talk about the geometry about a particular atom rather than the geometry of the molecule as a whole.
Larger Molecules

The structure of the whole molecule is only clear when we look at the whole molecule. But the geometry about each atom still follows the same rules!
Polarity

• In Chapter 8 we discussed bond dipoles.
• polar bonds versus polar molecules. We must think about the molecule as a whole.
Polarity

By adding the individual bond dipoles, one can determine the overall dipole moment for the molecule.
Polarity
“The tractor pull”
Overlap and Bonding

- Covalent bonds form when electrons are “shared.”
- But how, when the electrons are in these atomic orbitals? Do atomic orbitals overlap?
- Yes.
Overlap and Bonding

- Increased overlap brings the electrons and nuclei closer together while simultaneously decreasing electron-electron repulsion.
- However, if atoms get too close, the internuclear repulsion greatly raises the energy.
Hybrid Orbitals

But how do you get tetrahedral, trigonal bipyramidal, and other geometries when the atomic orbitals seem to be at right angles from each other all the time?
Hybrid Orbitals

• Consider beryllium:
  – In its ground electronic state, it would not be able to form bonds because it has no singly-occupied orbitals.
Hybrid Orbitals

But if it absorbs the small amount of energy needed to promote an electron from the 2s to the 2p orbital, it can form two bonds.
Hybrid Orbitals

- Mixing the $s$ and $p$ orbitals yields two degenerate orbitals that are hybrids of the two orbitals.
  - These $sp$ hybrid orbitals have two lobes like a $p$ orbital.
  - One of the lobes is larger and more rounded as is the $s$ orbital.
Hybrid Orbitals

• These two degenerate orbitals would align themselves 180° from each other.
• This is consistent with the observed geometry of beryllium compounds: linear.
Hybrid Orbitals

- With hybrid orbitals the orbital diagram for beryllium would look like this.
- The $sp$ orbitals are higher in energy than the 1s orbital but lower than the 2p.
Hybrid Orbitals

Using a similar model for boron leads to…

1↓ 1 1
2s 2p 2s 2p

Promote

Hybridize

sp² 2p
Hybrid Orbitals

...three degenerate $sp^2$ orbitals.
Hybrid Orbitals

With carbon we get…

\[ \begin{align*}
2s & \quad 2p \\
\rightarrow \quad \text{Promote} & \quad 1 \\
2s & \quad 2p \\
\rightarrow \quad \text{Hybridize} & \quad sp^3
\end{align*} \]
Hybrid Orbitals

...four degenerate $sp^3$ orbitals.
Hybrid Orbitals

For geometries involving expanded octets on the central atom, we must use $d$ orbitals in our hybrids.
Hybrid Orbitals

This leads to five degenerate $sp^3d$ orbitals…

…or six degenerate $sp^3d^2$ orbitals.
Hybrid Orbitals

Once you know the number of things around an atom, you know the hybridization state of the atom if you can count letters up to six.
Exam 3 topics

- Chapter 7, periodic properties
- Chapter 8, covalent and ionic bonding
- Chapter 8, electronegativity
- Chapter 8, polar bonds
- Chapter 8, Lewis structures
  - standard lewis structures
  - formal charge
  - resonance
  - less than an octet
  - more than an octet
- Chapter 9, geometry and shape of molecules
- Chapter 9, polarity/dipole moments of whole molecules
- Chapter 9, introduction to covalent bonding, diatomics
Exam 3 topics

• Chapter 9, hybridization sp, sp$^2$, sp$^3$, sp$^3$d, sp$^3$d$^2$
Chapter 7

- Periodic trends
- Effective nuclear charge
- Trends in atomic radius
- Trends in ion radius
- Ionization energy, trends
- Electron affinity, trends.
Effective Nuclear Charge

The effective nuclear charge, $Z_{\text{eff}}$, is:

$$Z_{\text{eff}} = Z - S$$

where $Z =$ atomic number  $S =$ screening constant, usually close to the number of inner (n-1) electrons.

\[ 
\begin{align*}
10- \quad \text{[Ne] core (10−)} \quad \text{Combined effect} = 11 - 10 = 1+ \\
11+ \quad \text{Nucleus (11+)}
\end{align*}
\]
Valence electrons:

How many valence electrons in:

O
O^2-
Co
Co^{2+}
Bonding atomic radius tends to...

...decrease from left to right across a row due to increasing $Z_{\text{eff}}$.

...increase from top to bottom of a column due to increasing value of $n$. 

Sizes of Atoms

Bonding atomic radius tends to...

...decrease from left to right across a row due to increasing $Z_{\text{eff}}$.

...increase from top to bottom of a column due to increasing value of $n$. 

Molecular Geometries and Bonding
**Sizes of Ions**

<table>
<thead>
<tr>
<th>Group 1A</th>
<th>Group 2A</th>
<th>Group 3A</th>
<th>Group 6A</th>
<th>Group 7A</th>
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</thead>
<tbody>
<tr>
<td>Li⁺</td>
<td>Li</td>
<td>Be²⁺</td>
<td>Be</td>
<td>B³⁺</td>
</tr>
<tr>
<td>0.68</td>
<td>1.34</td>
<td>0.31</td>
<td>0.90</td>
<td>0.23</td>
</tr>
<tr>
<td>Na⁺</td>
<td>Na</td>
<td>Mg²⁺</td>
<td>Mg</td>
<td>Al³⁺</td>
</tr>
<tr>
<td>0.97</td>
<td>1.54</td>
<td>0.66</td>
<td>1.30</td>
<td>0.51</td>
</tr>
<tr>
<td>K⁺</td>
<td>K</td>
<td>Ca²⁺</td>
<td>Ca</td>
<td>Ga³⁺</td>
</tr>
<tr>
<td>1.33</td>
<td>1.96</td>
<td>0.99</td>
<td>1.74</td>
<td>0.62</td>
</tr>
<tr>
<td>Rb⁺</td>
<td>Rb</td>
<td>Sr²⁺</td>
<td>Sr</td>
<td>In³⁺</td>
</tr>
<tr>
<td>1.47</td>
<td>2.11</td>
<td>1.13</td>
<td>1.92</td>
<td>0.81</td>
</tr>
</tbody>
</table>

Ionic size depends upon:
- Nuclear charge.
- Number of electrons.
- Orbitals in which electrons reside.
Trends in First Ionization Energies

On a smaller scale, there are two jags in each line. Why?
Trends in Electron Affinity

There are also two discontinuities in this trend.

<table>
<thead>
<tr>
<th>Element</th>
<th>Electron Affinity (eV)</th>
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<tr>
<td>H</td>
<td>-73</td>
</tr>
<tr>
<td>Li</td>
<td>-60</td>
</tr>
<tr>
<td>Be</td>
<td>&gt; 0</td>
</tr>
<tr>
<td>Na</td>
<td>-53</td>
</tr>
<tr>
<td>Mg</td>
<td>&gt; 0</td>
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<tr>
<td>K</td>
<td>-48</td>
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<tr>
<td>Ca</td>
<td>-2</td>
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<td>Rb</td>
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<td>C</td>
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<td>N</td>
<td>&gt; 0</td>
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<td>O</td>
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<td>F</td>
<td>-328</td>
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<td>Ne</td>
<td>&gt; 0</td>
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<td>Al</td>
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<td>Si</td>
<td>-134</td>
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<td>P</td>
<td>-72</td>
</tr>
<tr>
<td>S</td>
<td>-200</td>
</tr>
<tr>
<td>Cl</td>
<td>-349</td>
</tr>
<tr>
<td>Ar</td>
<td>&gt; 0</td>
</tr>
<tr>
<td>Ga</td>
<td>-30</td>
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<tr>
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<td>Te</td>
<td>-190</td>
</tr>
<tr>
<td>I</td>
<td>-295</td>
</tr>
<tr>
<td>Xe</td>
<td>&gt; 0</td>
</tr>
</tbody>
</table>
Exam 3 topics

- Chapter 8, covalent and ionic bonding
  - What is ionic bonding? What holds the atoms together?
  - Energetics of ionic bonding
  - Lattice energy
Exam 3 topics

• Chapter 8, electronegativity
  – What is electronegativity?
  – What are the trends on the periodic table?
• Chapter 8, polar bonds
Exam 3 topics

• Chapter 8, Lewis structures
  – standard lewis structures
  – formal charge
  – resonance
  – less than an octet
  – more than an octet

\[ \text{XeF}_2, \text{XeF}_6, \text{CO}_3^-, \text{NO}_2, \text{ClO}_4^-, \text{SbF}_5, \text{SO}_2, \text{SO}_3^{2-}, \text{H}_2\text{O}_2 \]
Exam 3 topics

- Chapter 8, bond enthalpies
  - use bond enthalpy table to calculate a $\Delta H$ of reaction
  - bonds broken - bonds made = enthalpy of reaction.
Exam 3 topics

• Chapter 9, geometry and shape of molecules, VSEPR.
• Chapter 9, polarity/dipole moments of whole molecules

• Give the geometry, shape and predict the dipole moment of each:

• XeF$_2$, ClO$_4^-$, SF$_4$, BrO$_2^-$
Exam 3 topics

Chapter 9, introduction to covalent bonding, diatomics

covalent bonds form when electrons are “shared.” But how, when the electrons are in these atomic orbitals? Do atomic orbitals overlap? Yes.

[Diagram showing bond formation between H and Cl atoms through overlap of 1s and 3p orbitals.]

Molecular Geometries and Bonding
Exam 3 answers

\[ \text{F—Xe—F } \quad \text{TBP, linear, nonpolar} \]

\[ \text{F—Br—F } \quad \text{octahedral, square pyramid, polar} \]

\[ \text{F—S—F } \quad \text{TBP, See saw, polar} \]
trigonal planar, trigonal planar, nonpolar
Exam 3

Note: 53 4 points (better than 80%)

<table>
<thead>
<tr>
<th>Bin</th>
<th>Frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
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<tr>
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</tr>
<tr>
<td>100</td>
<td>3</td>
</tr>
<tr>
<td>105</td>
<td>2</td>
</tr>
</tbody>
</table>

Mean 59.53774
Median 61.5
Mode 32
SD 21.4384
Range 101
Minimum 3
Maximum 104
Count 212
Regrade policy

• See your T.A. at recitation.
• Must be more than 7 points
• Entire exam will be regraded.
• We’re giving back points for direction of polarity on most of the problems where it is an issue BEFORE we give exam back.
• 12, 13, 15, 19, 20
• You only draw arrows for 2 problems.
Valence Bond Theory

- Hybridization is a major player in this approach to bonding.
- There are two ways orbitals can overlap to form bonds between atoms.
Sigma (\(\sigma\)) Bonds

- Sigma bonds are characterized by
  - Head-to-head overlap.
  - Cylindrical symmetry of electron density about the internuclear axis.
Pi ($\pi$) Bonds

- Pi bonds are characterized by
  - Side-to-side overlap.
  - Electron density above and below the internuclear axis.
Single Bonds

Single bonds are always $\sigma$ bonds, because $\sigma$ overlap is greater, resulting in a stronger bond and more energy lowering.

\[
\begin{align*}
\text{H–H} & \quad \text{One } \sigma \text{ bond} \\
\text{H} & \quad \text{H} \\
\text{C=\textcolor{blue}{\text{C}}} & \quad \text{One } \sigma \text{ bond plus one } \pi \text{ bond} \\
\text{H} & \quad \text{H} \\
\text{N=N} & \quad \text{One } \sigma \text{ bond plus two } \pi \text{ bonds}
\end{align*}
\]
Multiple Bonds

In a multiple bond one of the bonds is a $\sigma$ bond and the rest are $\pi$ bonds.
Multiple Bonds

• Example: formaldehyde an $sp^2$ orbital on carbon overlaps in $\sigma$ fashion with the corresponding orbital on the oxygen.

• The unhybridized $\rho$ orbitals overlap in $\pi$ fashion.
Multiple Bonds

In triple bonds, as in acetylene, two \( sp \) orbitals form a \( \sigma \) bond between the carbons, and two pairs of \( p \) orbitals overlap in \( \pi \) fashion to form the two \( \pi \) bonds.
Delocalized Electrons: Resonance

When writing Lewis structures for species like the nitrate ion, we draw resonance structures to more accurately reflect the structure of the molecule or ion.
Delocalized Electrons: Resonance

- each of the four atoms in the nitrate ion has a $p$ orbital.
- The $p$ orbitals on all three oxygens overlap with the $p$ orbital on the central nitrogen.
Delocalized Electrons: Resonance

This means the $\pi$ electrons are not localized between the nitrogen and one of the oxygens, but rather are delocalized throughout the ion.
The organic molecule benzene has six $\sigma$ bonds and a $p$ orbital on each carbon atom.
Resonance

- In reality the $\pi$ electrons in benzene are not localized, but delocalized.
- The even distribution of the $\pi$ electrons in benzene makes the molecule unusually stable.
Molecular Orbital (MO) Theory

Valence bond theory works very well for most observed properties of ions and molecules, but there are some concepts better represented by molecular orbital theory.
Molecular Orbital (MO) Theory

- In MO theory, we invoke the wave nature of electrons.
- If waves interact constructively, the resulting orbital is lower in energy: a bonding molecular orbital.
Molecular Orbital (MO) Theory

If waves interact destructively, the resulting orbital is higher in energy: an antibonding molecular orbital.
Molecular Orbital (MO) Theory

- Valence bond theory:
  - atomic orbitals are mixed in each individual atom before bonding.

- Molecular orbital theory:
  - no prebonding mixing. Molecular orbitals are computed after bonding.
MO Theory

- In $\text{H}_2$ the two electrons go into the bonding molecular orbital.
- The bond order is one half the difference between the number of bonding and antibonding electrons.
MO Theory

For hydrogen, with two electrons in the bonding MO and none in the antibonding MO, the bond order is

\[
\frac{1}{2} \ (2 - 0) = 1
\]
MO Theory

- In the case of He$_2$, the bond order would be
  \[
  \frac{1}{2} \ (2 - 2) = 0
  \]
- Therefore, He$_2$ does not exist.
Rules for making and filling molecular orbitals

• 1. The number of MO’s equals the # of Atomic orbitals
• 2. The overlap of two atomic orbitals gives two molecular orbitals, 1 bonding, one antibonding
• 3. Atomic orbitals combine with other atomic orbitals of similar energy.
• 4. Degree of overlap matters. More overlap means bonding orbital goes lower in E, antibonding orbital goes higher in E.
• 5. Each MO gets two electrons
• 6. Orbitals of the same energy get filled 1 electron at a time until they are filled.
MO Theory

- For atoms with both s and p orbitals, there are two types of interactions:
  - The s and the p orbitals that face each other overlap in \( \sigma \) fashion.
  - The other two sets of p orbitals overlap in \( \pi \) fashion.
• The resulting MO diagram looks like this.
• There are both s and p bonding molecular orbitals and s* and π* antibonding molecular orbitals.
MO Theory

- The earlier \( p \)-block elements in the second period have a sizeable interaction between the \( s \) and \( p \) orbitals.
- This flips the order of the \( \sigma \) and \( \pi \) molecular orbitals in these elements.
# Second-Row MO Diagrams

<table>
<thead>
<tr>
<th></th>
<th>Large 2s-2p interaction</th>
<th>Small 2s-2p interaction</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\text{B}_2$</td>
<td>$\text{C}_2$</td>
</tr>
<tr>
<td>$\sigma_{2p}^\sigma$</td>
<td>[ ]</td>
<td>[ ]</td>
</tr>
<tr>
<td>$\pi_{2p}^\sigma$</td>
<td>[ ]</td>
<td>[ ]</td>
</tr>
<tr>
<td>$\sigma_{2p}$</td>
<td>[ ]</td>
<td>[ ]</td>
</tr>
<tr>
<td>$\pi_{2p}$</td>
<td>[ ]</td>
<td>[ ]</td>
</tr>
<tr>
<td>$\sigma_{2s}^\sigma$</td>
<td>[ ]</td>
<td>[ ]</td>
</tr>
<tr>
<td>$\sigma_{2s}$</td>
<td>[ ]</td>
<td>[ ]</td>
</tr>
</tbody>
</table>

### Bond order
- $\text{B}_2$: 1
- $\text{C}_2$: 2
- $\text{N}_2$: 3
- $\text{O}_2$: 2
- $\text{F}_2$: 1
- $\text{Ne}_2$: 0

### Bond enthalpy (kJ/mol)
- $\text{B}_2$: 290
- $\text{C}_2$: 620
- $\text{N}_2$: 941
- $\text{O}_2$: 495
- $\text{F}_2$: 155
- $\text{Ne}_2$: 0

### Bond length (Å)
- $\text{B}_2$: 1.59
- $\text{C}_2$: 1.31
- $\text{N}_2$: 1.10
- $\text{O}_2$: 1.21
- $\text{F}_2$: 1.43
- $\text{Ne}_2$: 1.0
Heterodiatomic molecules

CO has a triple bond

C atom    CO molecule    O atom

Copyright © 2006 Pearson Prentice Hall, Inc.
Heterodiatomic molecules

NO is paramagnetic radical

N atom

NO molecule

O atom

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Why MO theory?

MO theory explains things that Valence Bond theory does not.

1. Magnetism
2. Color of molecules
3. Excited states of molecules.
Magnetism

We learned that electrons have magnetic quantum number $m_s$ “spin”.

Electrons have magnetic moment.

Electrons cause magnetism.

Three kinds of magnetism:

1. Diamagnetism
2. Paramagnetism
3. Ferromagnetism
Molecular Geometries and Bonding

Diamagnetic

(a) The sample is first weighed in the absence of a magnetic field.

N
S

(b) When a field is applied, a diamagnetic sample moves out of the field and thus appears to have a lower mass.

Paramagnetic

(c) A paramagnetic sample is drawn into the field and thus appears to gain mass.

Electrons all paired

Unpaired electrons

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Oxygen $\text{O}_2$ is Paramagnetic!

$\text{O} \equiv \text{O}$  Why?
### MO to the rescue

<table>
<thead>
<tr>
<th></th>
<th>Large $2s-2p$ interaction</th>
<th>Small $2s-2p$ interaction</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$B_2$</td>
<td>$C_2$</td>
</tr>
<tr>
<td>$\sigma^{\pm}_{2p}$</td>
<td><img src="image1" alt="Diagram" /></td>
<td><img src="image2" alt="Diagram" /></td>
</tr>
<tr>
<td>$\pi^{\pm}_{2p}$</td>
<td><img src="image7" alt="Diagram" /></td>
<td><img src="image8" alt="Diagram" /></td>
</tr>
<tr>
<td>$\sigma_{2p}$</td>
<td><img src="image13" alt="Diagram" /></td>
<td><img src="image14" alt="Diagram" /></td>
</tr>
<tr>
<td>$\pi_{2p}$</td>
<td><img src="image19" alt="Diagram" /></td>
<td><img src="image20" alt="Diagram" /></td>
</tr>
<tr>
<td>$\sigma^{\pm}_{2s}$</td>
<td><img src="image25" alt="Diagram" /></td>
<td><img src="image26" alt="Diagram" /></td>
</tr>
<tr>
<td>$\sigma_{2s}$</td>
<td><img src="image31" alt="Diagram" /></td>
<td><img src="image32" alt="Diagram" /></td>
</tr>
</tbody>
</table>

**Bond order**
- $B_2$: 1
- $C_2$: 2
- $N_2$: 3
- $O_2$: 2
- $F_2$: 1
- $Ne_2$: 0

**Bond enthalpy (kJ/mol)**
- $B_2$: 290
- $C_2$: 620
- $N_2$: 941
- $O_2$: 495
- $F_2$: 155
- $Ne_2$: —

**Bond length (Å)**
- $B_2$: 1.59
- $C_2$: 1.31
- $N_2$: 1.10
- $O_2$: 1.21
- $F_2$: 1.43
- $Ne_2$: —

**Magnetic behavior**
- $B_2$: Paramagnetic
- $C_2$: Diamagnetic
- $N_2$: Diamagnetic
- $O_2$: Paramagnetic
- $F_2$: Diamagnetic
- $Ne_2$: —
Ferromagnetism

Like iron, pulled to a magnet.

Long range order of spins in material

\[
\begin{array}{cccc}
S & & & \\
& S & & \\
& & S & \\
& & & S \\
N & & & \\
& N & & \\
& & N & \\
& & & N \\
\end{array}
\]
Remember, elements produced color because of electrons moving from higher to lower energy levels.

With MO theory, color of molecules is explained the same way.
Conjugated polyenes have MO’s that give rise to colors. Energy is absorbed, electrons go to higher energy levels.
How do we see color?

Isomerization wiggles the rest of the protein, sends nerve signal.

Rhodopsin

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How does Color Vision work?

Each rhodopsin (Rod, Blue, Green, Red) protein exhibits a different wavelength maxima as a result of 11\textit{cis}-retinal binding as a protonated Schiff base (PSB) via a lysine residue. It is these interactions that lead to color vision and allow us to see the whole visible spectrum.

11-\textit{cis}-retinal : \textasciitilde 380 nm
11-\textit{cis}-retinal SB : \textasciitilde 365 nm
11-\textit{cis}-retinal PSB : \textasciitilde 440 nm
PSB in Blue Rhodopsin : \textasciitilde 410 nm
PSB in Green Rhodopsin : \textasciitilde 530 nm
PSB in Red Rhodopsin : \textasciitilde 560 nm
PSB in Rod Rhodopsin : \textasciitilde 500 nm
You can change the energy of the MO’s of retinal by changing the environment around the molecule.