Drawing Lewis Structures

*The Octet Rule*

1. Determine the arrangement of atoms in the molecule
   - Some elements work only as terminal atoms (H, F, Cl, etc)
   - Some are particularly good as internal atoms (C, N)
2. Determine the total number of valence electrons in all atoms (don’t forget charge!)
   - Add numbers of all valence electrons
   - If negatively charged, add the appropriate number of electrons
   - If positively charged, subtract the appropriate number of electrons
3. Place one pair of electrons between each pair of bonded atoms, forming a bond
4. Use remaining electron pairs as lone pairs around each terminal atom, to complete its octet
5. Place electrons around the central atom. If you run out, “share” electron pairs from terminal atoms
Which is the best Lewis structure?

1) \[
\left[ \begin{array}{c}
: \text{C} \\
\equiv
\end{array} \right]
\]

2) \[
\left[ \begin{array}{c}
: \text{C} \\
\equiv
\end{array} \right]
\]

3) \[
\left[ \begin{array}{c}
: \text{C} \\
\text{N}
\end{array} \right]
\]
Which is the best Lewis structure?

1) $\begin{pmatrix} :C = = N:\ \end{pmatrix}$ 10 e⁻  
   C – [He]2s²2p²  
   N – [He]2s²2p³

2) $\begin{pmatrix} :C = = N:\ \end{pmatrix}$ 12 e⁻  
   Plus 1 e⁻  
   Too many electrons

3) $\begin{pmatrix} :C \rightleftharpoons N:\ \end{pmatrix}$ 14 e⁻  
   Too many electrons
Isoelectronic species
(10 electrons)

\[
\begin{align*}
\text{N} & \quad \text{C} \quad \text{O} \\
\text{N} & \quad \text{He}2s^22p^3 \quad \text{C} - \text{He}2s^22p^2 \quad \text{C} - \text{He}2s^22p^2 \\
\text{N} & \quad \text{He}2s^22p^3 \quad \text{O} - \text{He}2s^22p^4 \quad \text{N} - \text{He}2s^22p^3 \\
2+3+2+3 & \quad 2+2+2+4 \quad 2+2+2+3+1
\end{align*}
\]
Which is the best Lewis structure?

1) \[
\left[ \begin{array}{c}
:O \\ \equiv \\ N \\ \equiv \\ O:
\end{array} \right]^+ \quad 16 \text{ e}^-
\]

2) \[
\left[ \begin{array}{c}
:O \\ \equiv \\ N \\ \equiv \\ O:
\end{array} \right]^+ \quad 16 \text{ e}^-
\]

3) \[
\left[ \begin{array}{c}
:O \\ \equiv \\ N \\ \equiv \\ O:
\end{array} \right]^+ \quad 16 \text{ e}^-
Which is the best Lewis structure?

1) \[
\left[ \begin{array}{c}
:O \\ \leftrightarrow \\ N \\ \leftrightarrow \\ O:
\end{array} \right]^{+} 16 \text{ e}^{-}
\]

2) \[
\left[ \begin{array}{c}
:O \\ \leftrightarrow \\ N \\ \leftrightarrow \\ O:
\end{array} \right]^{+} 16 \text{ e}^{-}
\]

3) \[
\left[ \begin{array}{c}
:O \\ \leftrightarrow \\ N \\ \leftrightarrow \\ O:
\end{array} \right]^{+} 16 \text{ e}^{-}
\]

N \text{ – [He]2s}^{2}2p^{3}
O \text{ – [He]2s}^{2}2p^{4}
Minus 1 \text{ e}^{-}
Which is the best Lewis structure?

1) \([\text{O} = \text{N} = \text{O}]^+\) 16 e⁻

N – [He]2s²2p³
O – [He]2s²2p⁴

2) \([\text{O} = \text{N} = \text{O}]^+\) 16 e⁻

O – [He]2s²2p⁴

3) \([\text{O} \equiv \text{N} \equiv \text{O}]^+\) 16 e⁻

Minus 1 e⁻
Which is the best Lewis structure?

1) \[ \left[ \begin{array}{c} \text{O} \\ \text{N} \\ \text{O} \end{array} \right]^{+} \quad 16 \text{ e}^{-} \]

2) \[ \left[ \begin{array}{c} \text{O} \\ \text{N} \\ \text{O} \end{array} \right]^{+} \quad 16 \text{ e}^{-} \]

3) \[ \left[ \begin{array}{c} \text{O} \\ \text{N} \\ \text{O} \end{array} \right]^{+} \quad 16 \text{ e}^{-} \]

N – [He]2s²2p³
O – [He]2s²2p⁴

More than an octet

Less than an octet

Minus 1 e⁻
Move lone pairs to create double bonds and satisfy the octet for N.
Move lone pairs to create double bonds and satisfy the octet for N.
Move lone pairs to create double bonds and satisfy the octet for N.
Move lone pairs to create double bonds and satisfy the octet for N.

Remove an electron (any electron)
Move lone pairs to create double bonds and satisfy the octet for N.

\[ \text{Remove an electron (any electron)} \]
Move lone pairs to create double bonds and satisfy the octet for N.
Move lone pairs to create double bonds and satisfy the octet for N.
Move lone pairs to create double bonds and satisfy the octet for N.

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Move lone pairs to create double bonds and satisfy the octet for N.
Move lone pairs to create double bonds and satisfy the octet for N.
• Octet Rule - double count shared electrons
  – assumes both atoms get both electrons

\[
\begin{array}{cccc}
\text{O} & \equiv & \text{N} & \equiv & \text{O} \\
\end{array}
\]
• Octet Rule - double count shared electrons
  – assumes both atoms get both electrons

\[
\begin{array}{ccc}
8 & \equiv & 8 \\
\vdots & N & \equiv & \vdots \\
8 & \equiv & 8 \\
\end{array}
\]

Formal Charge
versus Octet Rule

• Octet Rule - double count shared electrons
  – assumes both atoms get both electrons

\[
\begin{array}{c}
\text{8} \\
\text{O} \equiv \text{N} \equiv \text{O} \\
\end{array}
\]

• Formal Charge - Evenly split electrons in a bond
  – one to one atom, one to the other

\[
\begin{array}{c}
\text{8} \\
\text{O} \equiv \text{N} \equiv \text{O} \\
\end{array}
\]
Formal Charge versus Octet Rule

• Octet Rule - double count shared electrons
  – assumes both atoms get both electrons
    \[ \boxed{\begin{array}{c}
    \text{8} \\
    \text{O} \equiv \text{N} \equiv \text{O}
    \end{array}} \] \(^+\)

• Formal Charge - Evenly split electrons in a bond
  – one to one atom, one to the other
    \[ \boxed{\begin{array}{c}
    \text{O} : \text{N} : \text{O}
    \end{array}} \] \(^+\)
Formal Charge

versus Octet Rule

• Octet Rule - double count shared electrons
  – assumes both atoms get both electrons

  \[
  \begin{array}{c}
  \text{O} \\
  \text{N} \\
  \text{O}
  \end{array}
  \]

• Formal Charge - Evenly split electrons in a bond
  – one to one atom, one to the other

  \[
  \begin{array}{c}
  \text{O} \\
  \text{N} \\
  \text{O}
  \end{array}
  \]
Formal Charge  
versus Octet Rule  

• Octet Rule - double count shared electrons  
  – assumes both atoms get both electrons  

\[
\begin{array}{c}
\text{O} \equiv \text{N} \equiv \text{O} \\
\end{array}
\]  

\[\text{8} \quad \text{8} \quad \text{8}\]  

• Formal Charge - Evenly split electrons in a bond  
  – one to one atom, one to the other  

\[
\begin{array}{c}
\text{O} \equiv \text{N} \equiv \text{O} \\
\end{array}
\]  

\[\text{6} \quad \text{4} \quad \text{6}\]  

\[\text{8} \quad \text{8} \quad \text{8}\]  

Brought to the party
Formal Charge versus Octet Rule

• Octet Rule - double count shared electrons
  – assumes both atoms get both electrons

\[
\begin{array}{c}
\text{O} \\
\text{N} \\
\text{O}
\end{array}
\]^{+}

• Formal Charge - Evenly split electrons in a bond
  – one to one atom, one to the other

\[
\begin{array}{c}
\text{6} \\
\text{O} \\
\text{N} \\
\text{O} \\
\text{6}
\end{array}
\]^{+}

Brought to the party
Formal Charge
versus Octet Rule

• Octet Rule - double count shared electrons
  – assumes both atoms get both electrons

\[ \begin{array}{c}
8 \\
\text{O} \equiv \text{N} \equiv \text{O}
\end{array} \]^{+}

• Formal Charge - Evenly split electrons in a bond
  – one to one atom, one to the other

\[ \begin{array}{c}
6 \\
\text{O} \\
\text{N} \\
\text{O}
\end{array} \]^{+}

Brought to the party

\[ \begin{array}{c}
6 \\
\text{O} \\
\text{N} \\
\text{O}
\end{array} \]
Formal Charge
versus Octet Rule

• Octet Rule - double count shared electrons
  – assumes both atoms get both electrons

\[
\left[ \begin{array}{c}
\text{O} \\
\text{N} \\
\text{O}
\end{array} \right]^+
\]

• Formal Charge - Evenly split electrons in a bond
  – one to one atom, one to the other

\[
\left[ \begin{array}{c}
\text{O} \\
\text{N} \\
\text{O}
\end{array} \right]^+
\]

Brought to the party

\[
\left[ \begin{array}{c}
\text{O} \\
\text{N} \\
\text{O}
\end{array} \right]^+
\]

\[
\text{O} \\
\text{N}
\]

12
Formal Charge versus Octet Rule

• Octet Rule - double count shared electrons
  – assumes both atoms get both electrons

\[
\begin{align*}
\text{O} & \equiv \text{N} \equiv \text{O} \\
8 & \quad 8 & \quad 8 \\
\end{align*}
\]

• Formal Charge - Evenly split electrons in a bond
  – one to one atom, one to the other

\[
\begin{align*}
\text{O} & \equiv \text{N} \equiv \text{O} \\
6 & \quad 4 & \quad 6 \\
\end{align*}
\]
Formal Charge

versus Octet Rule

Number of electrons brought to the party

Number of electrons ending up with

Brought to the party

Formal Charge

Ends up with

6

4

6

+1

0

0

6

5

6

6

5

Ends up with one fewer than it “came with” or wants, so N has a formal charge of +1
Formal Charge versus Octet Rule

Number of electrons brought to the party

Number of electrons ending up with

Note: sum of atom formal charges must equal the overall charge on the molecule
Formal Charge

versus Octet Rule

Number of electrons brought to the party

Number of electrons ending up with

Note: sum of atom formal charges must equal the overall charge on the molecule
Formal charge = \(-1 = 6 - \left[6 + \frac{1}{2}(2)\right]\)

Formal charge = \(+2 = 7 - \left[2 + \frac{1}{2}(6)\right]\)
Formal charge = $-1 = 6 - \left[ 6 + \frac{1}{2}(2) \right]$
Formal charge = \(-1\) = \(6 - \left[6 + \frac{1}{2}(2)\right]\)

\[
\begin{array}{c}
\vdots \\
:0: \\
\vdots \\
\vdots \\
\vdots \\
:0&-\text{Cl}&-0:
\end{array}
\]

Formal charge = \(+2\) = \(7 - \left[2 + \frac{1}{2}(6)\right]\)
Formal charge = \(-1 = 6 - [6 + \frac{1}{2}(2)]\)

\[
\begin{array}{c}
\text{Cl} \\
\end{array}
\]

\[
\begin{array}{c}
\text{O} \\
\end{array}
\]

Formal charge = \(+2 = 7 - [2 + \frac{1}{2}(6)]\)

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Formal charge $= -1 = 6 - [6 + \frac{1}{2}(2)]$

$7 - 5 = +2$

Formal charge $= +2 = 7 - [2 + \frac{1}{2}(6)]$
Formal charge $= -1 = 6 - \left[ 6 + \frac{1}{2}(2) \right]$
Formal charge = \( -1 = 6 - [6 + \frac{1}{2}(2)] \)

\[
\begin{array}{c}
0 \\
\text{Cl} \\
0
\end{array}
\]

Formal charge = \( +2 = 7 - [2 + \frac{1}{2}(6)] \)

\(-1 = +2 - 3(-1)\)
Formal charge $= -1 = 6 - [6 + \frac{1}{2}(2)]$

Sum of formal charges $= -1$

Formal charge $= 0 = 1 - [0 + \frac{1}{2}(2)]$
New concept: Oxidation Number
New concept

\[
\left[ \begin{array}{c}
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\end{array} \right. \quad \begin{array}{c}
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\end{array} \\
\end{array} \end{array}
\right]^{-}
New concept

\[
\left[ \overset{\text{O}}{\underset{\text{H}}{\text{O}}} \right]^-
\]

\[
\left[ \overset{\text{O}}{\underset{\text{H}}{\text{O}}} \right]^-
\]

Formal Charge

Covalent assumption

Electrons shared, one to each
New concept

$\left[ \begin{array}{c} \text{O} \\
\vdots \\
\text{H} 
\end{array} \right]^{-}$

$\left[ \begin{array}{c} \text{O} \\
\vdots \\
\text{H} 
\end{array} \right]^{-}$  $\left[ \begin{array}{c} \text{O} \\
\vdots \\
\text{H} 
\end{array} \right]^{-}$

**Formal Charge**

Covalent assumption

Electrons shared, one to each

**Oxidation Number**

Ionic assumption

Both electrons transferred to the one who wants them more
Assume an ionic bond

\[
\begin{array}{c}
\text{Oxidation number } = -2 \\
\text{Sum of oxidation numbers } = -1 \\
\text{Oxidation number } = +1
\end{array}
\]
Formal charge $= -1 = 6 - [6 + \frac{1}{2}(2)]$

$\left[ \begin{array}{c} \vdots \\ O \\ \vdots \\ \vdots \\ H \end{array} \right]^{-} \quad \text{Sum of formal charges} = -1$

Formal charge $= 0 = 1 - [0 + \frac{1}{2}(2)]$

$\left[ \begin{array}{c} \vdots \\ \vdots \\ \vdots \\ O \\ \vdots \\ H \end{array} \right]^{-} \quad \text{Sum of oxidation numbers} = -1$

Assume an ionic bond

Oxidation number $= -2$

Oxidation number $= +1$
Formal charge $= -1 = 6 - [6 + \frac{1}{2}(2)]$

$\text{Sum of formal charges} = -1$

Formal charge $= 0 = 1 - [0 + \frac{1}{2}(2)]$

Oxidation number $= -2$

$\text{Sum of oxidation numbers} = -1$

Assume an ionic bond

Oxidation number $= +1$
**Octet Rule - double count** shared electrons

— assumes both atoms get both electrons
• **Octet Rule - double count** shared electrons
  — assumes both atoms get both electrons

• **Formal Charge - *Evenly*** split electrons in a bond
  — one to one atom, one to the other
- **Octet Rule - double count** shared electrons
  - assumes both atoms get both electrons
- **Formal Charge - *Evenly*** split electrons in a bond
  - one to one atom, one to the other
- **Oxidation Number - *Unevenly*** split electrons in a bond
  - the atom that wants electrons more, gets both shared electrons (as in ionic bonds). The other one loses out. *An extreme view.*
Questions?
Back to Octet Rule
Ozone anion \( \text{O}_3^- \)

Alternative Ways of Drawing the Ozone Structure

Double bond on the left: \( \text{O} = \text{O} - \text{O} : \)

Double bond on the right: \( : \text{O} - \text{O} = \text{O} \)

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Ozone anion \( \text{O}_3^- \)

**Alternative Ways of Drawing the Ozone Structure**

Double bond on the left: \[ \text{O} = \text{O} - \text{O} : \]

Double bond on the right: \[ : \text{O} - \text{O} = \text{O} \]

Which side gets the double bond?
Real molecule - equal bond lengths!! (not interconverting)
Nitrite anion - NO$_2^-$

Formal charge =
\[
0 = 6 - [4 + \frac{1}{2}(4)]
\]

Formal charge =
\[
-1 = 6 - [6 + \frac{1}{2}(2)]
\]

\[
[\begin{array}{c}
O \\
\\nN \\
\\
O
\end{array}]^{-}
\]

Formal charge = 0 = 5 - [2 + \frac{1}{2}(6)]
Nitrite anion - NO$_2^-$

Formal charge = 
\[0 = 6 - [4 + \frac{1}{2}(4)]\]

Formal charge = 
\[-1 = 6 - [6 + \frac{1}{2}(2)]\]

Resonance Structure - two views; neither fully correct

\[
\begin{array}{c}
\text{O} \equiv \text{N} \equiv \text{O} \\
\end{array}
\]

\[
\begin{array}{c}
\text{O} \equiv \text{N} \equiv \text{O} \\
\end{array}
\]
Nitrite anion - \( \text{NO}_2^- \)

Unified Structure - one view; more correct

Resonance Structure - two views; neither fully correct
Nitrite anion - NO$_2^-$

**Unified Structure - one view; more correct**

\[
\begin{array}{c}
\text{O} \\
\text{N} \\
\text{O}
\end{array}
\]

But harder to implement the octet rule

**Resonance Structure - two views; neither fully correct**

\[
\begin{array}{c}
\text{O} \\
\text{N} \\
\text{O}
\end{array} \quad \leftrightarrow \quad \begin{array}{c}
\text{O} \\
\text{N} \\
\text{O}
\end{array}
\]
Exceeding the Octet Rule
using near-energy d orbitals

5x7 = 35 electrons brought to the party

The last two electron pairs are added to the central Cl atom.
<table>
<thead>
<tr>
<th>Group 4A</th>
<th>Group 5A</th>
<th>Group 6A</th>
<th>Group 7A</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₄</td>
<td>NH₃</td>
<td>H₂O</td>
<td>HF</td>
</tr>
<tr>
<td>methane</td>
<td>ammonia</td>
<td>water</td>
<td>hydrogen fluoride</td>
</tr>
<tr>
<td>C₂H₆</td>
<td>N₂H₄</td>
<td>H₂O₂</td>
<td></td>
</tr>
<tr>
<td>ethane</td>
<td>hydrazine</td>
<td>hydrogen peroxide</td>
<td></td>
</tr>
<tr>
<td>C₂H₄</td>
<td>NH₄⁺</td>
<td>H₃O⁺</td>
<td></td>
</tr>
<tr>
<td>ethylene</td>
<td>ammonium ion</td>
<td>hydronium ion</td>
<td></td>
</tr>
<tr>
<td>C₂H₂</td>
<td>NH₂⁻</td>
<td>OH⁻</td>
<td></td>
</tr>
<tr>
<td>acetylene</td>
<td>amide ion</td>
<td>hydroxide ion</td>
<td></td>
</tr>
</tbody>
</table>

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