Worksheet 14 - Lewis structures

Determine the Lewis structure of $O_2$ oxygen gas.

1. Complete the Lewis dot symbols for the oxygen atoms below
   \[ \text{O} \quad \text{O} \]

2. Determine the number of **valence electrons** available in the $O_2$ molecule.
   \[
   \text{total valence electrons} = \text{6} + \text{6} = 12
   \]
   Use two of these electrons to make a **bond** between the 2 oxygen atoms.
   \[ \text{O} : \text{O} \]

3. Determine the number of **unused valence electrons.** \[10\]

4. Place the remaining electrons as **pairs of electrons** around the $O_2$ structure.
   \[ \text{O} : \text{O} \]
   Does each of the O atoms have an **octet** of electrons? \[\text{No}\]

Use **lone pair electrons** to make an additional bond between the O atoms.
   \[ \text{O} :: \text{O} \]
   Does each of the O atoms have an **octet** of electrons? \[\text{Yes}\]

Oxygen gas consists of 2 oxygen atoms, joined by a **double bond**, O=O. Each oxygen atom has two lone pairs of electrons.

**Rules for Lewis Structures**

1) Count the valence electrons that you have to work with.

2) Put the least electronegative atom in the center (except H)

3) Use pairs of electrons to form bonds between all atoms

4) Use remaining electrons to complete octets.

5) If you run out of electrons, introduce multiple bonds to get octets.
5. Determine the Lewis structure of CO₂, carbon dioxide.

a) Total valence electrons = \( 4 + 6 + 6 = 16 \text{e}^- \)

b) Place the least electronegative atom in the center of the molecule and use pairs of electrons to bond the 3 atoms

\[ \text{O} : \text{C} : \text{O} \]

c) \# of remaining electrons = \( 12 + 4 = 16 \text{e}^- \)

Place these in pairs around the atoms. Do all of the atoms have octets? O=C=O

Move lone pair electrons until every atom has 8 valence electrons.

Draw the bonding of CO₂.

\[ \text{C doesn't have octet C shell doesn't have octet} \]

6. Determine the Lewis structure for N₂, nitrogen gas, then draw its bonding.

\[ \text{N} : \text{N} \]

7. Determine the Lewis structure for nitric acid, HNO₃. Hydrogen can never be in the middle of a compound and can only have 2 valence electrons, giving it the noble gas structure of He. The acidic hydrogen is bonded to oxygen.

\[ 1 + 5 + 3(r) = 24 \text{e}^- \]

\[ \text{O} = \text{N} - \text{O} - \text{H} \]

The structure of HNO₃ illustrates the idea of resonance, one O has a single bond to N and the other has a double bond. SO₂, sulfur dioxide, whose Lewis structure is shown below, also exhibits resonance. The Lewis structure shows one single and one double bond.

\[ \text{O} : \text{S} : \text{O} \]

In fact, both S-O bonds are identical. This is shown below, where the double error indicates that the two structures are equivalent.

\[ \text{:O:S:O} \quad \leftrightarrow \quad \text{O::S::O} \]
New structures generated by the movement of electron pairs are called resonance structures.

Draw the resonance structure for HNO₃ in problem 7.

\[
\begin{align*}
\text{O} & \equiv \text{N} - \text{O} - \text{H} \\
& \leftrightarrow \\
\text{O} & \equiv \text{N} - \text{O} - \text{H}
\end{align*}
\]

8. Draw the Lewis structure for the carbonate ion, CO₃²⁻. The negative charge indicates that there are additional electrons in this structure. Draw all possible resonance structures of carbonate.

Exception to the Octet Rule

1. **Species with odd numbers of electrons**

   The gas, NO, has 11 valence electrons and can not be described by using a Lewis structure.

2. **Species with fewer than 8 valence electrons**

   Boron tends to form compounds with fewer than 8 valence electrons. For example BF₃ can be described as

   \[
   \begin{align*}
   \text{B} & \equiv \text{F} - \text{F} - \text{F} \\
   \text{B} & \equiv \text{F} - \text{F} - \text{F}
   \end{align*}
   \]

   *It is found that BF₃ is very reactive with species containing lone pair electrons, like ammonia, NH₃. (Draw the Lewis structure of NH₃). The lone pair on nitrogen forms a coordinate covalent bond with B, with both bonding electrons coming from N. This is also called a Lewis Acid/Base reaction, which we will discuss in more detail later.*

3. **Species with Expanded Shells**

   These species have more than 8 electrons around the central atom. These structures are only possible when the principal quantum number is greater than n = 3 and d orbitals are available for bonding. These are most common with large central atoms bonded to small, electronegative atoms.
Formal Charge

When more than one resonance structure is possible, the determination of the best structure can be made based on the formal charges in the structure. The calculation of the formal charge is given by:

\[
\text{formal charge} = \text{# valence electrons} - \frac{1}{2} \text{shared electrons} - \text{lone pair electrons}
\]

We determined that the structure of BF₃ is an exception to the octet rule:

\[
\begin{align*}
\text{BF}_3 & \quad \text{valence \varepsilon}_{\text{on B}} = 3 - \frac{1}{2} \times 6 \quad \text{bonding \varepsilon} - 0 \quad \text{lone pair \varepsilon} = 0 \\
\text{valence \varepsilon}_{\text{on F}} & = 7 - \frac{1}{2} \times 2 \quad \text{bonding \varepsilon} - 6 \quad \text{lone pair \varepsilon} = 0
\end{align*}
\]

We could draw a different resonance structure by moving lone pair electrons:

\[
\begin{align*}
\text{BF}_3 & \quad \text{valence \varepsilon}_{\text{on B}} = 3 - \frac{1}{2} \times 6 \quad \text{bonding \varepsilon} - 0 \quad \text{lone pair \varepsilon} = 0 \\
\text{valence \varepsilon}_{\text{on F}} & = 7 - \frac{1}{2} \times 2 \quad \text{bonding \varepsilon} - 6 \quad \text{lone pair \varepsilon} = 0
\end{align*}
\]

The octet rule is obeyed, but this is not the structure of BF₃. To see why it is not, determine the formal charges of B and F in this second structure. The formal charges are non-zero and there is a positive charge on the most electronegative element, F. The best resonance structures have the smallest possible formal charges, and negative charges on electronegative elements.

9. Draw the Lewis structure of COCl₂.

a) What is the central atom? C

b) How many valence electrons are available? 4 + 6 = 10

c) Draw all three possible resonance structures:

\[
\begin{align*}
\text{COCl}_2 & \quad \text{Cl} & \quad \text{O} & \quad \text{C} & \quad \text{Cl} \\
\text{O} & \quad \text{Cl} & \quad \text{C} & \quad \text{O} & \quad \text{Cl}
\end{align*}
\]

d) Assign formal charges in each and decide which is the best structure.

\[
\text{Cl} - \text{O} - \text{Cl} \quad \text{best structure} \quad \text{no formal charges}
\]
10. Draw the Lewis structure for phosphorus pentachloride.
   a) What is the formula? \( \text{PCl}_5 \)
   b) How many valence electrons are available? \( 5(7) + 5 = 40e^- \)
   c) Place the P in the center and make 5 bonds to Cl
      \[ \begin{array}{c}
      \text{Cl} \\
      \text{P} \\
      \text{Cl}
      \end{array} \]
   d) Complete the octets on the Cl atoms
   e) How many electrons remain? 30
   f) Place lone pairs of electrons on P if necessary. How many lone pairs are on P? none

11. Draw the Lewis structure for xenon tetrafluoride
   a) What is the formula? \( \text{XeF}_4 \)
   b) How many valence electrons are available? \( 8 + 4(7) = 36e^- \)
   c) Place the Xe in the center and make 4 bonds to F
      \[ \begin{array}{c}
      \text{F} \\
      \text{F} \\
      \text{Xe} \\
      \text{F}
      \end{array} \]
   d) Complete the octets on the F atoms
   e) How many electrons remain? 4e-
   f) Place lone pairs of electrons on Xe, if necessary. How many lone pairs are on Xe? 2 lone pairs

12. Phosphorus and nitrogen are both in Group V. \( \text{PCl}_3 \) and \( \text{PCl}_5 \) both exist. \( \text{NCl}_3 \) exists, but \( \text{NCl}_5 \) is an unstable compound. Why?

   \[ \begin{align*}
   \text{P} &; n = 3 \\
   \text{N} &; n = 2
   \end{align*} \]

   \( \text{PCl}_3 \) and \( \text{PCl}_5 \) can have 5 Cl bonded to it (extended octet)

   \( \text{NCl}_3 \) can have 5 Cl bonded to it (extended octet)
13. Fill in the Lewis dot symbols for H, C, N, O and Cl. Based on this information predict how many bonds and how many lone pairs each of these atoms will possess.

<table>
<thead>
<tr>
<th>element</th>
<th>Lewis symbol</th>
<th>bonds</th>
<th>lone pairs</th>
</tr>
</thead>
<tbody>
<tr>
<td>hydrogen</td>
<td>H.</td>
<td>1</td>
<td>none</td>
</tr>
<tr>
<td>carbon</td>
<td>.C.</td>
<td>1</td>
<td>none</td>
</tr>
<tr>
<td>nitrogen</td>
<td>.N.</td>
<td>3</td>
<td>1</td>
</tr>
<tr>
<td>oxygen</td>
<td>.O.</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>chlorine</td>
<td>.Cl.</td>
<td>1</td>
<td>3</td>
</tr>
</tbody>
</table>

14. Based on your results in question 13, complete the structure of Tylenol, drawn below. Show all multiple bonds and lone pairs.

15. Draw Lewis structures for:

a) \( \text{PO}_4^{3-} \) \( 5 + 4(6) + 3 = 32e^- \)

b) \( \text{ClO}_3^- \) \( 7 + 3(6) + 1 = 26e^- \)

c) \( \text{OF}_2 \) \( 6 + 14 = 20e^- \)

d) \( \text{CO} \) \( 6 + 4 = 10e^- \)
16. Draw Lewis structures for the following compounds. If they exhibit resonance, draw all of the resonance structures.

a) \( \text{XeO}_2\text{F}_2 = 8 + 2(6) + 2(7) = 34e^- \)

\[
\begin{align*}
\text{Xe} & \quad \text{O} & \quad \text{F} \\
\text{O} & \quad \text{F} & \quad \text{Xe} & \quad \text{F} \\
\text{O} & & & & \text{O} \\
\end{align*}
\]

b) \( \text{NO}_2 \quad 5 + 2(6) + 1 = 18e^- \)

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

c) \( \text{C}_2\text{H}_4 \quad 2(4) + 4(1) = 12e^- \)

\[
\begin{align*}
\text{H} & \quad \text{H} & \quad \text{C} & \quad \text{H} & \quad \text{H} \\
\text{H} & \quad \text{C} & \quad \text{H} & \quad \text{H} & \quad \text{H} \\
\end{align*}
\]

d) \( \text{SO}_3 \quad 6 + 3(6) = 24e^- \)

\[
\begin{align*}
\text{O} & \quad \text{S} & \quad \text{O} & \quad \text{O} \\
\text{O} & \quad \text{S} & \quad \text{O} & \quad \text{O} \\
\end{align*}
\]

e) \( \text{SCl}_6 \quad 6(7) = 48e^- \)

\[
\begin{align*}
\text{S} & \quad \text{Cl} & \quad \text{Cl} & \quad \text{Cl} & \quad \text{Cl} & \quad \text{Cl} \\
\text{Cl} & \quad \text{Cl} & \quad \text{Cl} & \quad \text{Cl} & \quad \text{Cl} \\
\end{align*}
\]

f) \( \text{KrF}_2 \quad 8 + 2(7) = 22e^- \)

\[
\begin{align*}
\text{F} & \quad \text{Kr} & \quad \text{F} \\
\text{F} & \quad \text{Kr} & \quad \text{F} \\
\end{align*}
\]

17. Draw three resonance structures of \( \text{N}_2\text{O} \), in which the atoms are arranged in the order N  N  N  O. Indicate the formal charges in each.