Name: ____________________________

**Answer Key: Shapes of Molecules**

**Background**
The valence shell electron pair repulsion (VSEPR) theory is how the geometry of a molecule is determined. It’s called “vesper” theory for short. The shapes that are possible are tetrahedral, trigonal planar, trigonal pyramidal, bent, and linear. To determine the shape of a molecule, you must look at the central atom. Though only atoms and not unbonded electrons are considered when naming the shape of a molecule, the unbonded electrons are still very important because they do affect the location of the outer atoms around the central atom, and therefore the shape of the molecule. Unbonded electrons around atoms that are not the central atom have little effect on the geometry.

In this activity, you will draw Lewis structures for a number of substances and use them to determine how the molecular models need to be assembled. From the models, you will determine the geometry of the substance. After completing a few examples, you should start to see how the two dimensional drawings really exist in three dimensions.

**Procedure**
Complete each column in order. Compare your model to the samples at the front of the room if you are confused about which geometry your model makes.

<table>
<thead>
<tr>
<th>Substance (write the chemical formula)</th>
<th>Total Valence (e^-)</th>
<th>Lewis structure (check the box if a resonance structure is possible)</th>
<th>Lewis structure with proper geometry (use the models to help here)</th>
<th>VSEPR geometry (the name of the shape)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water (\text{H}_2\text{O})</td>
<td>(2(1) + 6 = 8)</td>
<td><img src="image" alt="Lewis structure" /></td>
<td><img src="image" alt="Lewis structure" /></td>
<td>Bent</td>
</tr>
<tr>
<td>Nitrogen (\text{N}_2)</td>
<td>(2(5) = 10)</td>
<td><img src="image" alt="Lewis structure" /></td>
<td><img src="image" alt="Lewis structure" /></td>
<td>Linear</td>
</tr>
<tr>
<td>Molecule</td>
<td>Electron Count</td>
<td>Shape</td>
<td></td>
<td></td>
</tr>
<tr>
<td>--------------------------</td>
<td>----------------</td>
<td>------------------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Carbonate $\text{CO}_3^{2-}$</td>
<td>$4 + 3(6) + 2 = 24$</td>
<td>Trigonal planar</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sulfite* $\text{SO}_3^{2-}$</td>
<td>$6 + 3(6) + 2 = 26$</td>
<td>Trigonal pyramidal</td>
<td></td>
<td></td>
</tr>
<tr>
<td>*See note at the end of the document</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Carbon tetrachloride $\text{CCl}_4$</td>
<td>$4 + 4(7) = 32$</td>
<td>Tetrahedral</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ammonium $\text{NH}_4^+$</td>
<td>$5 + 4(1) - 1 = 8$</td>
<td>Tetrahedral</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Compound</td>
<td>Electron Count</td>
<td>Lewis Structure</td>
<td>Molecular Shape</td>
<td></td>
</tr>
<tr>
<td>------------------------</td>
<td>----------------</td>
<td>-----------------</td>
<td>-----------------</td>
<td></td>
</tr>
<tr>
<td>Bromine ( \text{Br}_2 )</td>
<td>14</td>
<td>![Lewis structure of Br₂]</td>
<td>Linear</td>
<td></td>
</tr>
<tr>
<td>Carbon monoxide ( \text{CO} )</td>
<td>10</td>
<td>![Lewis structure of CO]</td>
<td>Linear</td>
<td></td>
</tr>
<tr>
<td>Dinitrogen monoxide* ( \text{N}_2\text{O} )</td>
<td>16</td>
<td>![Lewis structure of N₂O]</td>
<td>Linear</td>
<td></td>
</tr>
<tr>
<td>Ozone ( \text{O}_3 )</td>
<td>18</td>
<td>![Lewis structure of O₃]</td>
<td>Bent</td>
<td></td>
</tr>
<tr>
<td>Anion</td>
<td>Electron Count</td>
<td>Traditional Count</td>
<td>Valence Shell Electron Dot Structure</td>
<td>Molecular Shape</td>
</tr>
<tr>
<td>-----------</td>
<td>----------------</td>
<td>-------------------</td>
<td>-------------------------------------</td>
<td>-----------------</td>
</tr>
<tr>
<td><strong>Nitrate</strong> $\text{NO}_3^-$</td>
<td>5 + 3(6) + 1 = <strong>24</strong></td>
<td>✓</td>
<td><img src="image1" alt="Nitrate structure diagram" /></td>
<td><strong>Trigonal planar</strong></td>
</tr>
<tr>
<td><strong>Nitrite</strong> $\text{NO}_2^-$</td>
<td>5 + 2(6) + 1 = <strong>18</strong></td>
<td>✓</td>
<td><img src="image2" alt="Nitrite structure diagram" /></td>
<td><strong>Bent</strong></td>
</tr>
<tr>
<td><strong>Bromate</strong> $\text{BrO}_3^-$</td>
<td>7 + 3(6) + 1 = <strong>26</strong></td>
<td><img src="image3" alt="Bromate structure diagram" /></td>
<td><strong>Trigonal pyramidal</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Chlorite</strong> $\text{ClO}_2^-$</td>
<td>7 + 2(6) + 1 = <strong>20</strong></td>
<td><img src="image4" alt="Chlorite structure diagram" /></td>
<td><strong>Bent</strong></td>
<td></td>
</tr>
</tbody>
</table>
### Analysis

Without using the models, determine the geometry of these substances (you can draw Lewis structures to help you):

<table>
<thead>
<tr>
<th>Substance</th>
<th>Geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>NF₃</td>
<td>Tetrahedral</td>
</tr>
<tr>
<td>H₂S</td>
<td>Bent</td>
</tr>
<tr>
<td>OCl₂</td>
<td>Bent</td>
</tr>
<tr>
<td>HCN</td>
<td>Linear</td>
</tr>
<tr>
<td>F₂</td>
<td>Linear</td>
</tr>
<tr>
<td>SO₂ *</td>
<td>Bent</td>
</tr>
<tr>
<td>SO₄²⁻ *</td>
<td>Tetrahedral</td>
</tr>
<tr>
<td>ClO₃⁻ *</td>
<td>Trigonal pyramidal</td>
</tr>
<tr>
<td>SO₃ (not sulfite!) *</td>
<td>Trigonal planar</td>
</tr>
</tbody>
</table>

**Phosphate**

PO₄³⁻

\[5 + 4(6) + 3 = 32\]

Tetrahedral

**Acetic Acid**

\(\text{CH}_3\text{COOH} \text{ (or} \ C_2H_4O_2\text{)}\)

\[2(4) + 4(1) + 2(6) = 24\]

N/A

(Tetrahedral around one carbon, Trigonal planar around the other carbon, bent around the oxygen between C and H)
Conclusion

All of the substances in this exercise have what kind of bonds? Explain why this is important.

All of the substances have covalent bonds, whether in a molecule or a polyatomic ion. This is important because if they were ionic compounds with ionic bonds, they would form a crystal lattice and they would not have individual molecules and so wouldn’t form any of these shapes.

A note on formal charges: Assigning formal charges to atoms in a covalently bonded molecule or ion is a way to keep track of electron distribution in that substance. Minimizing formal charges generally means a more stable structure, as low formal charges indicate that the electrons are relatively evenly distributed among the atoms in that substance. Additionally, it is more favorable to have negative formal charges on the atoms with higher electronegativities. The formal charge is calculated by starting with the initial number of valence electrons at atom would have and subtracting how many it “has” in the molecule, counting each electron in a lone pair as 1, and 1 of the electrons in any bonded pairs. The formula for calculating formal charge can be written like this:

\[
\text{Formal charge} = \text{valence electrons} - [\text{lone pair electrons} + \frac{1}{2}(\text{bonding electrons})]
\]

*These compounds have Lewis structures that work following the octet rule, but they also have other possible structures that violate the octet rule in order to have lower formal charges for the atoms in the substance. Sometimes, this leads to resonance structures that would not have been present with the Lewis structure that followed the octet rule. They do not change the geometry of the molecule or ion, as there are the same number of bonding regions around the central atom – some of the bonds just changed from single to double bonds with additional electrons coming from lone pairs on the outer atoms. These structures are included below, in the order they appeared in the worksheet. In the first examples, sulfite and dinitrogen monoxide, the formal charges for both versions are worked out so that you can see the difference between the structures.
**Sulfite:**

Original answer:

Sulfur: \( FC = 6 - [2 + \frac{1}{2}(6)] = 6 - (2 + 3) = 6 - 5 = +1 \)
Oxygens: \( FC = 6 - [6 + \frac{1}{2}(2)] = 6 - (6 + 1) = 6 - 7 = -1 \)

**Sulfur has +1 formal charge and all oxygens have −1**

Formal charges reduced:

Sulfur: \( FC = 6 - [2 + \frac{1}{2}(8)] = 6 - (2 + 4) = 6 - 6 = 0 \)
Single Bond oxygen: same as original
Double Bond oxygen: \( FC = 6 - [4 + \frac{1}{2}(4)] = 6 - (4 + 2) = 6 - 6 = 0 \)

**Sulfur and double bonded oxygen have 0 formal charge and single bonded oxygens have −1.**

This version is favorable because some of the atoms have a formal charge of 0 and the others didn’t change.

**Dinitrogen monoxide:**

For this one, there are no additional Lewis structures that can be formed, but the formal charge can tell you which one of the resonance structures is most favorable.

**Formal charges for Lewis structure 1:**
Left nitrogen: \( FC = 5 - [2 + \frac{1}{2}(6)] = 5 - (2 + 3) = 5 - 5 = 0 \)
Middle nitrogen: \( FC = 5 - [0 + \frac{1}{2}(8)] = 5 - 4 = +1 \)
Oxygen: \( FC = 6 - [6 + \frac{1}{2}(2)] = 6 - (6 + 1) = 6 - 7 = -1 \)

**Formal charges for Lewis structure 2:**
Left nitrogen: \( FC = 5 - [4 + \frac{1}{2}(4)] = 5 - (4 + 2) = 5 - 6 = -1 \)
Middle nitrogen: same as before
Oxygen: \( FC = 6 - [4 + \frac{1}{2}(4)] = 6 - (4 + 2) = 6 - 6 = 0 \)

**Formal charges for Lewis structure 3:**
Left nitrogen: \( FC = 5 - [6 + \frac{1}{2}(2)] = 5 - (6 + 1) = 5 - 7 = -2 \)
Middle nitrogen: FC = same as before
Oxygen: \( FC = 6 - [2 + \frac{1}{2}(6)] = 6 - (2 + 3) = 6 - 5 = +1 \)

Structure 1 is most favorable, as it minimizes the formal charges and, unlike structure 2, the negative formal charge is on the more electronegative atom (oxygen). Structure 2 is the second most favorable (because although charges are still +1 and −1, the negative formal charge is on the less electronegative atom, nitrogen), and structure 3 is least favorable because all atoms have a formal charge and in this one the left nitrogen has a larger (−2) formal charge than the others, which only have charges of ±1.
**Bromate:**
Original answer: \[
\begin{array}{c}
\text{Original answer:} \\
\text{Formal charges reduced:}
\end{array}
\]

**Chlorite:**
Original answer: \[
\begin{array}{c}
\text{Original answer:} \\
\text{Formal charges reduced:}
\end{array}
\]

**Phosphate:**
Original answer: \[
\begin{array}{c}
\text{Original answer:} \\
\text{Formal charges reduced:}
\end{array}
\]

**SO\textsubscript{2}:**
Original answer: \[
\begin{array}{c}
\text{Original answer:} \\
\text{Formal charges reduced:}
\end{array}
\]

**SO\textsubscript{4}\textsuperscript{2-}:**
Original answer: \[
\begin{array}{c}
\text{Original answer:} \\
\text{Formal charges reduced:}
\end{array}
\]

**ClO\textsubscript{3}\textsuperscript{-}:**
Original answer: \[
\begin{array}{c}
\text{Original answer:} \\
\text{Formal charges reduced:}
\end{array}
\]

**SO\textsubscript{3}:**
Original answer: \[
\begin{array}{c}
\text{Original answer:} \\
\text{Formal charges reduced:}
\end{array}
\]