Computing Formal Charges

• formal charge (fc) = (# valence e\(^-\)) – (# of bonds + # of unshared e\(^-\))

• In a neutral molecule, the sum of the formal charges is zero. For an ion, the sum of the formal charges is equal to the charge of the ion.

• An atom in a Lewis structure that has the number of bonds expected on the basis of its group number has no formal charge.

“Normal” covalent bonding patterns:

- Carbon
- Nitrogen
- Oxygen
- Halogen

<table>
<thead>
<tr>
<th>Bond Type</th>
<th>Example</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>One bond</td>
<td>One bond</td>
<td>One bond</td>
</tr>
<tr>
<td>Three lone pairs</td>
<td>Three lone pairs</td>
<td>Three lone pairs</td>
</tr>
<tr>
<td>Two bonds</td>
<td>Two bonds</td>
<td>Two bonds</td>
</tr>
<tr>
<td>One lone pair</td>
<td>One lone pair</td>
<td>One lone pair</td>
</tr>
<tr>
<td>Four bonds</td>
<td>Four bonds</td>
<td>Four bonds</td>
</tr>
<tr>
<td>No lone pairs</td>
<td>No lone pairs</td>
<td>No lone pairs</td>
</tr>
</tbody>
</table>

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Computing Formal Charges

- Common structures with formal charges:

<table>
<thead>
<tr>
<th>Carbon</th>
<th>Nitrogen</th>
<th>Oxygen</th>
<th>Halogens</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{\textsuperscript{+}C} )</td>
<td>( \text{\textsuperscript{+}N} )</td>
<td>( \text{\textsuperscript{-}O} )</td>
<td>( \text{\textsuperscript{-}X} )</td>
</tr>
<tr>
<td>( \text{\textsuperscript{-}N} )</td>
<td>( \text{\textsuperscript{-}N} )</td>
<td>( \text{\textsuperscript{-}O} )</td>
<td>( \text{\textsuperscript{-}X} )</td>
</tr>
</tbody>
</table>

Common structures with formal charges:

- The elements are arranged in the periodic table so that those with similar chemical properties are arranged in the same vertical column, called a **group** or a family.
- Each horizontal row is called a **period**.
Lewis structures indicate how the atoms within a molecule are connected, whether the bonds are single, double, or triple, and the locations of the extra, or non-bonding electrons. However, by themselves, Lewis structures do not provide any information about the three-dimensional shape of the molecule.

VSEPR Theory

The [valence-shell electron-pair repulsion theory](#), or VSEPR, enables us to predict the three-dimensional shape of a molecule from the completed Lewis structure of the molecule. This theory is based upon the idea that all of the pair of electrons on a central atom in a molecule will repel each other and try to get as far apart as possible. This includes both the bonding pairs of electrons and the non-bonding pairs on the atom.
We will first consider a series of molecules which possess no non-bonding electrons:

BeCl₂ (beryllium chloride) is an electron-deficient compound possessing two bonding pairs of electrons and no non-bonding pairs.

The two pairs of bonding electrons will be as far apart as possible if the bonds point in exactly opposite directions (180° apart).

This molecule is linear.

AlCl₃ (aluminum chloride) is an electron-deficient compound possessing three bonding pairs of electrons and no non-bonding pairs.

The three pairs of bonding electrons will be as far apart as possible if the bonds point at angles of 120° to each other.

This molecule is trigonal planar or triangular planar.

CH₄ (methane) possesses four bonding pairs of electrons and no non-bonding pairs.

Four pairs of electrons can get as far apart in space as possible if the four bonds point an angles in space of 109.5° to each other.

The shape of the methane molecule is tetrahedral.
In molecules such as water, \( \text{H}_2\text{O} \), and ammonia, \( \text{NH}_3 \), non-bonding as well as bonding electrons surround the central atom.

The non-bonding electrons and bonding electrons as a group will repel each other and will point in directions in space to try to get as far apart as possible.

The non-bonding electrons require a slightly larger volume in space than do the bonding electrons and, as a result, cause the angles between the bonding electrons to be slightly smaller than one might otherwise predict.

When applying the VSEPR theory to molecules containing non-bonding electrons, the shape of the molecule is determined by the positions of the outer atoms only. The positions of these outer atoms and the bond angles are determined by considering all of the electrons, both bonding and non-bonding.
NH₃ (ammonia) contains three bonding pairs of electrons and one non-bonding pair.

![Ammonia structure](image)

The four pairs of electrons will point in space in the directions of a regular tetrahedron, however, the shape of the molecule is named from the positions of the hydrogen atoms only, ignoring the lone pair of electrons. The shape of ammonia is called a **trigonal pyramid**.

H₂O (water) contains two bonding pairs of electrons and two non-bonding pairs.

![Water structure](image)

The four pairs of electrons will point in space in the directions of a regular tetrahedron, however, the shape of the molecule is named from the positions of the hydrogen atoms only, ignoring the lone pair of electrons. The shape of water is called **bent** or **angular**.
THREE-DIMENSIONAL MOLECULAR STRUCTURES

Rules for predicting molecular shape by VSEPR theory

- Determine the Lewis structure.
- Determine the number of electron pairs (bonded and nonbonded) surrounding a central atom.
- Use VSEPR theory to decide what symmetrical three-dimensional shape will accommodate all bonded and nonbonded electron pairs.
- Classify the shape of the molecule by considering the arrangement of the joined atoms only, ignoring the nonbonded electron pairs.

That is why, although the CH₄, NH₃, and H₂O molecules each have four pairs of electrons around the central atom, the shape of methane is tetrahedral, that of ammonia is trigonal pyramidal, and that of water is bent.

Atomic Orbitals

- $s$ orbital

- $p$ orbitals
  - $p_x$
  - $p_y$
  - $p_z$
Bonding in Organic Compounds

• Generate *hybrid orbitals* by “mixing” atomic orbitals in order to achieve the VSEPR geometries.

Methane

• VSEPR theory suggests a tetrahedral structure:

```
        H
       / \  
      H   C   H
     /   \  /   
    H     H   H
```
Methane

- VSEPR theory suggests a tetrahedral structure:

- But, the atomic orbitals on carbon do not have the correct geometry to give a tetrahedron.

Methane

- However, mixing the carbon 2s orbital and the 3 carbon 2p orbitals gives 4 $sp^3$ hybrid orbitals:
Methane

• However, mixing the carbon 2s orbital and the 3 carbon 2p orbitals gives 4 sp³ hybrid orbitals:

![Diagram of sp³ hybrid orbitals]

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Methane

• These 4 sp³ hybrid orbitals point toward the corners of a tetrahedron:

![Diagram of a tetrahedron with sp³ hybrid orbitals]

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Methane

• Orbital overlap of the carbon $sp^3$ with the hydrogen $1s$ orbitals gives the four $\sigma$ bonds:

\[ \text{A tetrahedral atom has } sp^3 \text{ hybridization.} \]

Ethene

• The molecular orbitals of ethene:
  – $1s$ orbitals of the four hydrogen atoms
  – $2s$, $2p_x$, $2p_y$, and $2p_z$ orbitals of the two carbon atoms
Ethene

• The $2s$, $2p_x$, and $2p_y$ orbitals on carbon form three $sp^2$ hybrid orbitals on each carbon atom.
• The three $sp^2$ hybrid orbitals point toward the corners of a triangle.

A trigonal planar atom has $sp^2$ hybridization.

Ethene

• The $sp^2$ hybrids and the $1s$ orbitals on hydrogen make up the $\sigma$-framework—$\sigma$ bonds that are relatively strong bonds.

A trigonal planar atom has $sp^2$ hybridization.
Ethene

• A weaker bond is formed that is made up entirely from the remaining 2p_z orbitals of the two carbon atoms overlapping in a $\pi$ bond.

Carbon Dioxide

• VSEPR theory suggests what type of structure?

$$O=C=O$$
Carbon Dioxide

- VSEPR theory suggests a linear structure:
  \[ \text{O} \equiv \text{C} \equiv \text{O} \]
- Mix a C 2s orbital and a C 2p orbital to give two \( sp \) hybrid orbitals that point in opposite directions:
  \[ \text{O} \quad \text{C} \quad \text{O} \]
- \( \pi \) bonds complete the bonding picture:

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

*A linear atom has \( sp \) hybridization.*

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