**VSEPR Theory**

**Predicting drawing and explaining the shapes of molecules**

The shapes of molecules can be predicted from their **Lewis structures** by using the **VSEPR** (**V**alence **S**hell **E**lectron **P**air **R**epulsion) theory. This theory states that electron groups around a central atoms will assume a geometry (shape) that keeps them as far apart from each other as possible.

An electron group can be a non-bonding pair of electrons, a bonding pair of electrons (in a single bond), a bonding quartet ( 2 pairs of e-s in a double bond), or a bonding sextet (3 pairs of e-s in a triple bond).

To predict the shape of a molecule…

* Draw a correct Lewis diagram for the molecule
* Count the electron **groups** (see above for the definition of electron group)
* Check against the table below

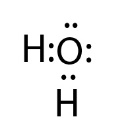
This is illustrated by the drawings and explanations below.

|  |  |  |  |
| --- | --- | --- | --- |
| Number of electron groups in molecule and  Description | | 3D image | 2 D sketch  **(bonds vs non-bonding pairs)** |
| **4** | **Four electron groups** surrounding a central atom will form a **tetrahedron**. All of the angles in a tetrahedron are **109.5o**, and all positions are equivalent. |  | **4** bonding groups of e-s **(CH4)**  **(TETRAHEDRON SHAPE)**  **3** bonding groups of e-s**, 1** non-bonding group of e-s **(NH3, NF3 )**  **(TRIGONAL PYRAMID SHAPE)**  **2** bonding groups of e-s, **2** non-bonding groups of e-s **(H2O)**  **(BENT SHAPE)** |
| **3** | **Three electron groups** surrounding a central atom will form a flat triangle (**trigonal planar**). Each of the angles is **120o** and all positions are equivalent. |  | **3** bonding groups**, 0** non-bonding groups.  **(TRIGONAL PLANAR)**  **BCl3**  **Carbon cpds with 1 dbl bond and 2 single bonds around the C atom, eg:**  **H2CO** (4 bonding pairs but only 3 bonding groups, as 2 pairs are in the same double bond) |
| **2** | **Two electron groups** surrounding a central atom form a straight line (**linear**) with **180o** between them |  | **H2**  **O2**  **CO2**  **H2C2** |

\*\* *(high level)* Non-bonding pairs of electrons are held closer to the central atom (as they are not shared or attracted to another atom), so a non-bonding pair of electrons effectively repels the other electron groups **more**. This is why the angles on some molecules based of a tetrahedral shape, but with non-bonding pairs (like H2O) have angles between bonds of less than 109.5o.

**So What? Why knowing about shape is important.**

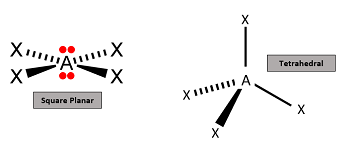
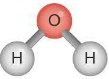
The arrangement of the pairs of electrons and the shape of the molecule can be used to draw inferences about the distribution of electrons within the molecule, and this can have significant impact on the strength of the intermolecular forces. Molecules which have unsymmetrical shapes often have lower than expected dispersion forces because the molecules cannot “pack” closely together. Molecules with uneven distribution of electrons within the molecule will have a molecular dipole, and thus have Dipole-Dipole intermolecular forces.



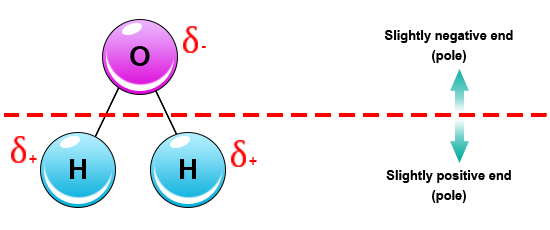
**Guided practice**

1. Draw the Lewis structure for water, H2O.

**four**

* 1. How many "groups"(atoms and lone pairs) surround the central oxygen?
  2. What is the **geometry** of this molecule (look at atoms and lone pairs)? Draw this VSEPR structure next to the Lewis structure.

**tetrahedral**

* 1. What is the **shape** of this molecule (look only at the atoms)?
  2. What is the H-O-H bond angle?

**104.5o**

* 1. *Place the partial positive and negative charges on the H and O atoms, based on their relative electronegativities. Is water a* ***polar*** *compound?*

**Polar**

1. Draw the Lewis structure for NH3.
   1. How many "groups"(atoms and lone pairs) surround the central nitrogen?
   2. What is the **geometry** of this molecule (look at atoms and lone pairs)? Draw this VSEPR structure next to the Lewis structure.
   3. What is the **shape** of this molecule (look only at the atoms)?
   4. What is the H-N-H bond angle?
   5. *Place the partial positive and negative charges on the N and O atoms, based on their relative electronegativities. Is NH3 a* ***polar*** *compound?*

Draw the Lewis and VSEPR structures for the following compounds and label them with their **geometry**.

**Lewis** **Diagram** **VSEPR shape** **Name of shape**

* 1. **CF4**
  2. **H2S**

**c) CO2**

**d) BH3**

**e) H3CCl**

**f) H2S**