Topic:	**Molecular Shape:** **VSEPR Theory (V**alence-**S**hell **E**lectron-**P**air **R**epulsion**)**
Objective:	**FK_03_04**

Given a molecule
the student must be capable of doing the following:

- **determine its Lewis structure**
- **determine its shape and bond angles**

VSEPR Theory

The Lewis structure of a molecule is a flat drawing showing

- the relative placement of parts (atoms),
- the connections (groups of bonding electrons, covalent bonds), and
- lone pairs of electrons.

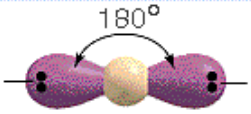
To construct the molecular shape from the Lewis structure, chemists employ **valence-shell electron-pair repulsion (VSEPR)** theory. Its basic principle is that **each group of electrons** (valence electrons) **around a central atom is located as far away from the others as possible in order to minimize repulsions**.

This group of electrons could be shared pairs of electrons (two electrons in the case of a single bond, four electrons in the case of a double bond or six electrons if a triple bond is formed) or a lone pair.

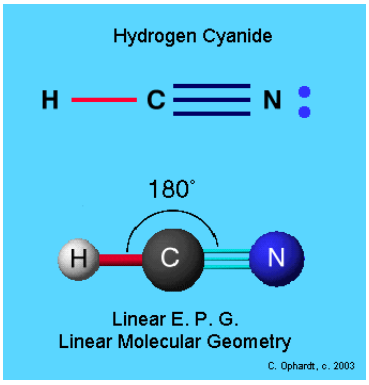
The Molecular Shape with Two Electron Groups (Linear Arrangement)

When two electron groups attached to a central atom are oriented as far as possible, they point in opposite directions. This linear arrangement of electron groups results in a **linear** molecular shape and a bond angle of 180°.

ELECTRON-PAIR GEOMETRIES AS A FUNCTION OF THE NUMBER OF ELECTRON PAIRS

Number of Electron Pairs	Arrangement of Electron Pairs	Electron-Pair Geometry	Predicted Bond Angles
2		Linear	180°

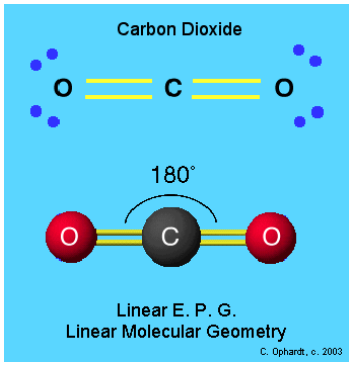
http://www.800mainstreet.com/5/0005-000-vsepr.gif



In the case of hydrogen cyanide we have two electron groups: the first group has two electrons (H-C bond) and the second group has six electrons (C ≡ N triple bond).

The molecule is **linear**.

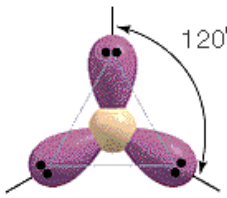
Carbon dioxide has the same shape, linear (two groups of electrons; each group having four electrons).



Molecular Shapes with Three Electron Groups (Trigonal Planar Arrangement)

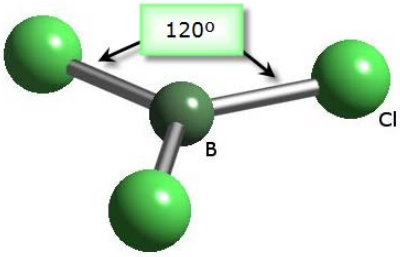
Three electron groups around the central atom repel each other to the corners of an equilateral triangle, which gives the **trigonal planar** arrangement.

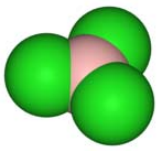
ELECTRON-PAIR GEOMETRIES AS A FUNCTION OF THE NUMBER OF ELECTRON PAIRS

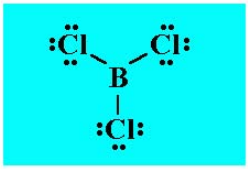
Number of Electron Pairs	Arrangement of Electron Pairs	Electron-Pair Geometry	Predicted Bond Angles
3		Trigonal planar	120°

When the three electron groups are bonding groups, the molecular shape is also trigonal planar (**AX_3**; A=Central atom, X=Surrounding atom)

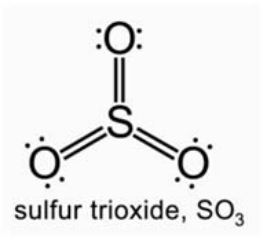
Boron trichloride is a trigonal planar molecule:

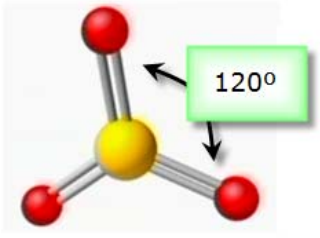


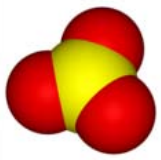




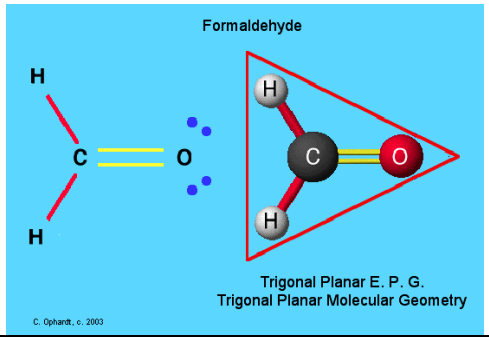
Sulphur trioxide molecule has the same shape:







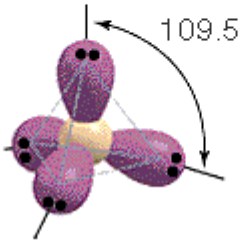
Formaldehyde molecule is also trigonal planar.



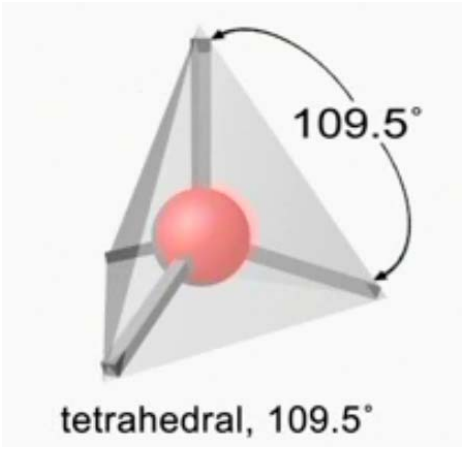
Molecular Shapes with Four Electron Groups (Tetrahedral Arrangement)

The shapes described so far have all been easy to depict in two dimensions, but four electron groups must use three dimensions to achieve maximal separation.

ELECTRON-PAIR GEOMETRIES AS A FUNCTION OF THE NUMBER OF ELECTRON PAIRS

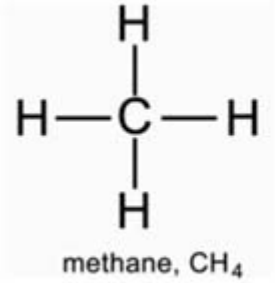
Number of Electron Pairs	Arrangement of Electron Pairs	Electron-Pair Geometry	Predicted Bond Angles
4		Tetrahedral	109.5°

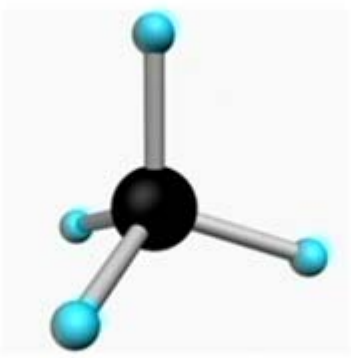
All molecules with four electron groups around a central atom adopt the **tetrahedral arrangement**.

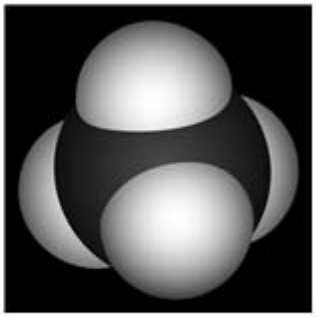


When all four electron groups are bonding groups, as in the case of methane, the **molecular shape is also tetrahedral** (**AX_4**).

Methane has a bond angle of 109.5º

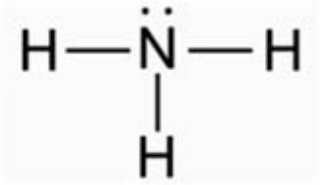


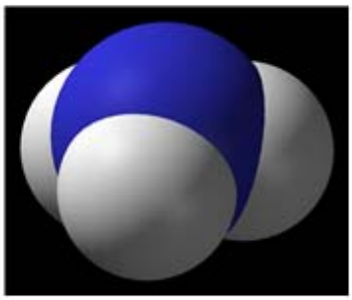




When one of the four electron groups in the tetrahedral arrangement is a lone pair, the molecular shape is that of a **trigonal pyramid** (**AX_3E**; A=central atom, X=surrounding atom, E=lone pair).

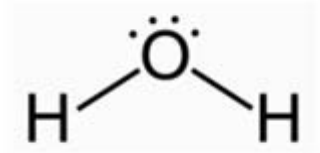
In ammonia (NH_3) the lone pair forces the N-H bonding pairs closer, and the H-N-H angle is 107.3º

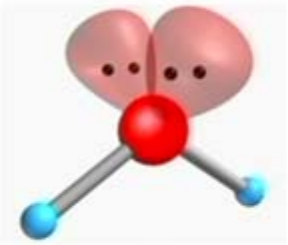


When the four electron groups around the central atom include two bondings and two nonbonding groups (**AX_2E_2**; A=central atom, X=surrounding atom, E=lone pair), the molecular shape is **bent** or **V shaped**.

Water is the most important V-shaped molecule in the tetrahedral arrangement.

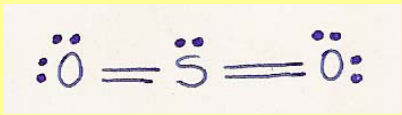




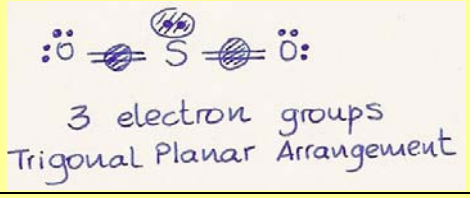

Determine the Lewis structure and the molecular shape of the following compounds

SO_2

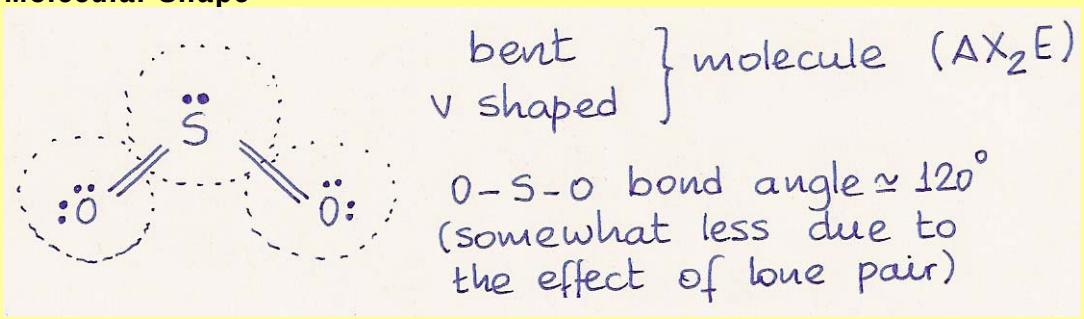
Lewis



Arrangement of Electron Pairs



Molecular Shape



BCl_3

Lewis

Arrangement of Electron Pairs

Molecular Shape

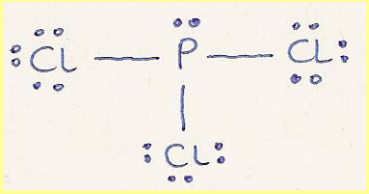
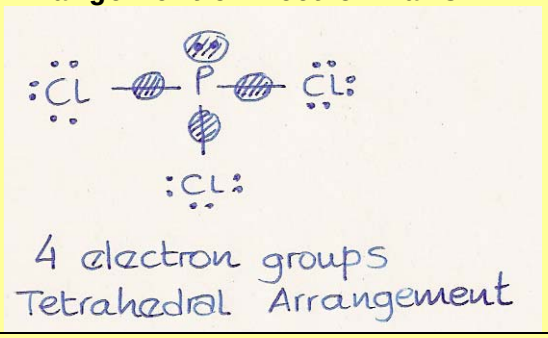
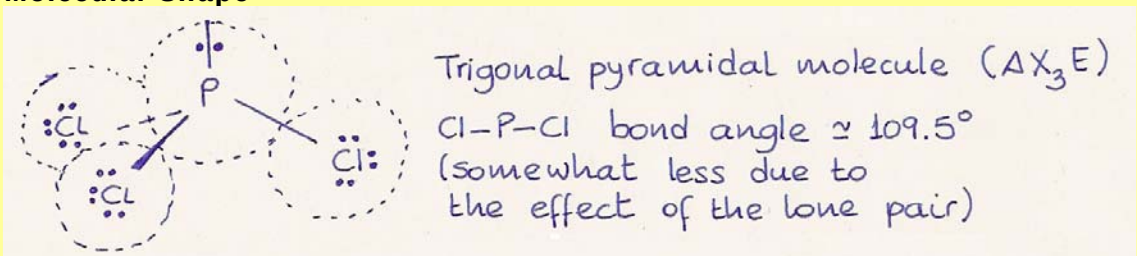
$CHCl_3$

Lewis

Arrangement of Electron Pairs

Molecular Shape

H_2CO	**Lewis**	**Arrangement of Electron Pairs**
	Molecular Shape	
HCN	**Lewis**	**Arrangement of Electron Pairs**
	Molecular Shape	
CO_2	**Lewis**	**Arrangement of Electron Pairs**
	Molecular Shape	

<table>
<tr><td rowspan="2">PCl_3</td><td>Lewis
  </td><td>Arrangement of Electron Pairs
 
4 electron groups
Tetrahedral Arrangement</td></tr>
<tr><td colspan="2">Molecular Shape
 
Trigonal pyramidal molecule (AX_3E)
Cl–P–Cl bond angle ≃ 109.5°
(somewhat less due to
the effect of the lone pair)</td></tr>
<tr><td rowspan="2">H_2O</td><td>Lewis</td><td>Arrangement of Electron Pairs</td></tr>
<tr><td colspan="2">Molecular Shape</td></tr>
<tr><td rowspan="2">NH_3</td><td>Lewis</td><td>Arrangement of Electron Pairs</td></tr>
<tr><td colspan="2">Molecular Shape</td></tr>
</table>