Chemical Bond DIARY

[Physics and Chemistry 1 DIARY] [Chemical Bonds Index] [Chemical Bond SEQUENCING] [Physics and Chemistry Sequencing]

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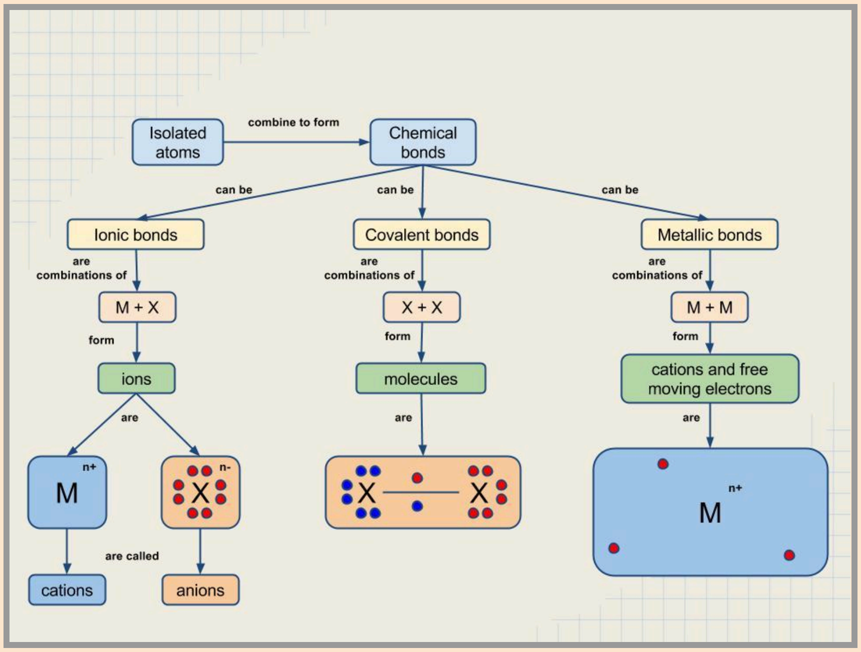
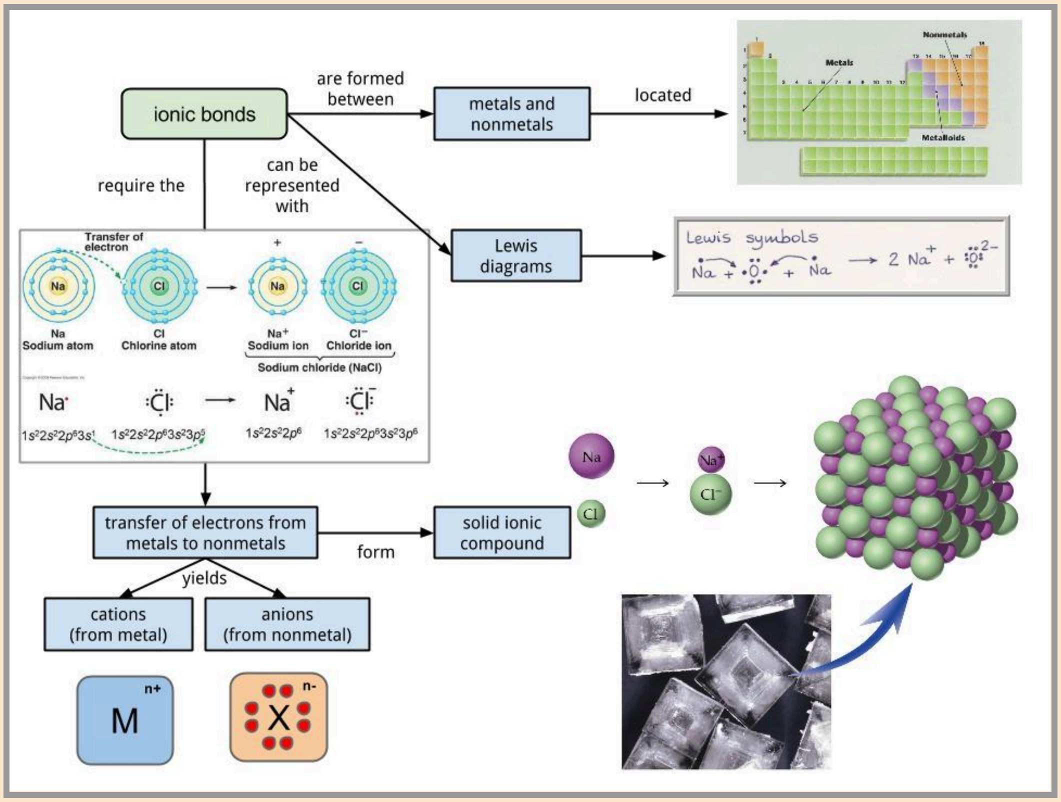
Session 01. Chemical Bond. Types of bonding. Ionic Bond. [Chemical Bonding - Some Conceptual Maps] [Formation of ionic bonds]





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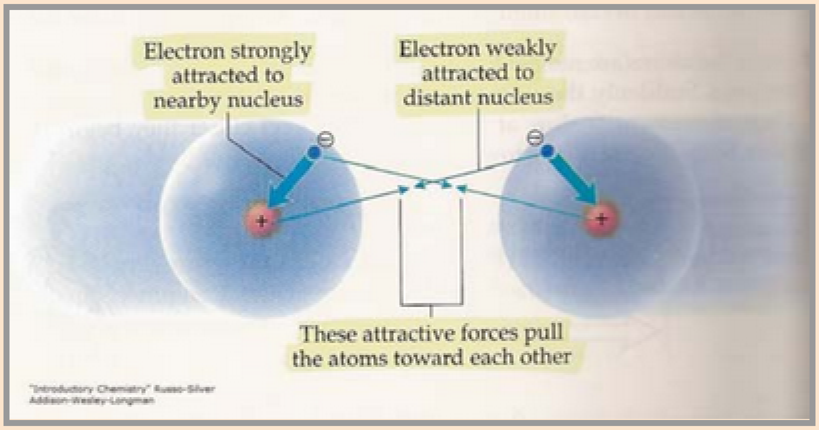
Session 02. Covalent Bond. [Covalent Bonds - Solutions to Exercises] [Homework: Exercises and solutions]

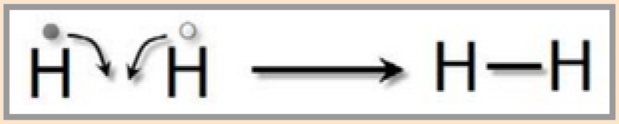
FORMATION OF COVALENT BONDS

In covalent bonds electrons are shared between atoms of nonmetals. When atoms approach each other, additional forces appear between electrons and the nucleus of the other atom.

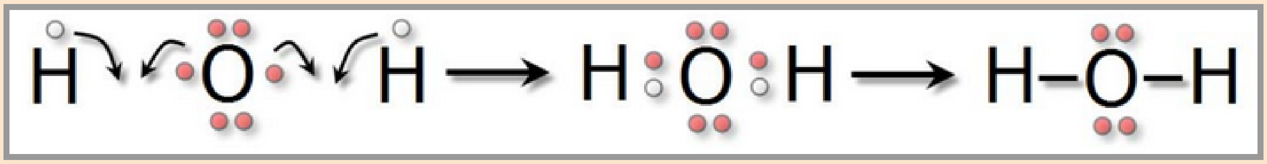


We can describe the formation of covalent bond in these equivalent ways:

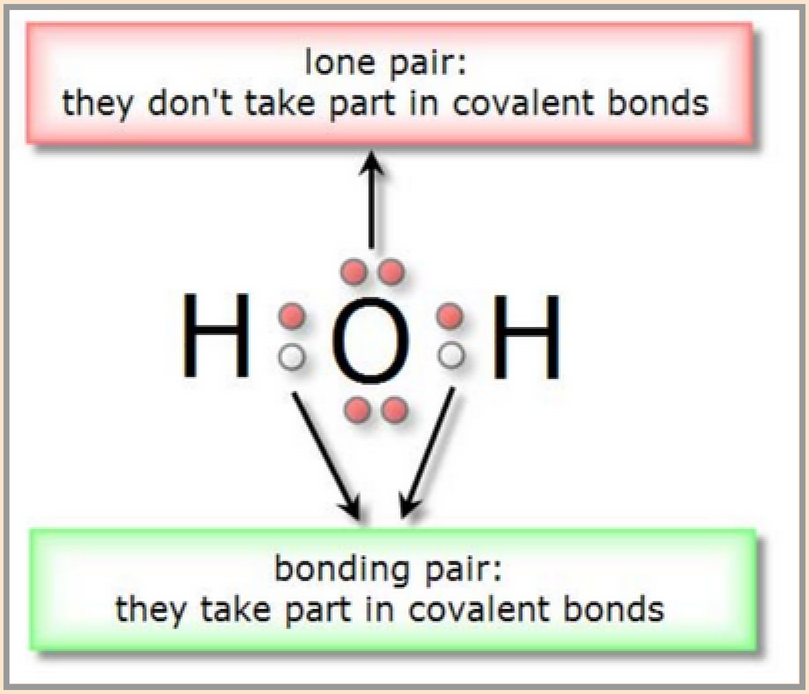
or



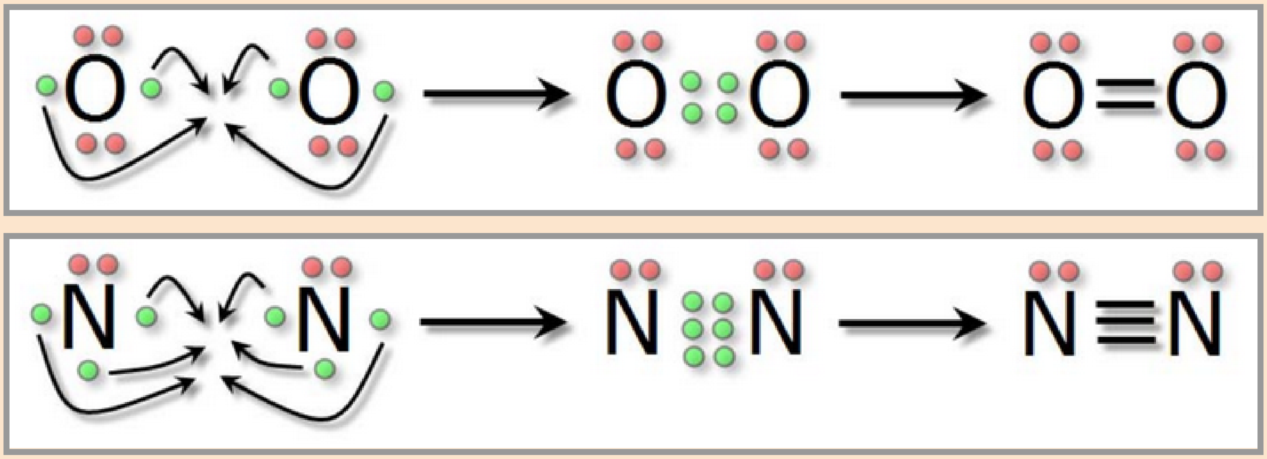
Only unpaired electrons are shared between atoms:



Paired electrons do not take part in bonds and they are called lone pairs:

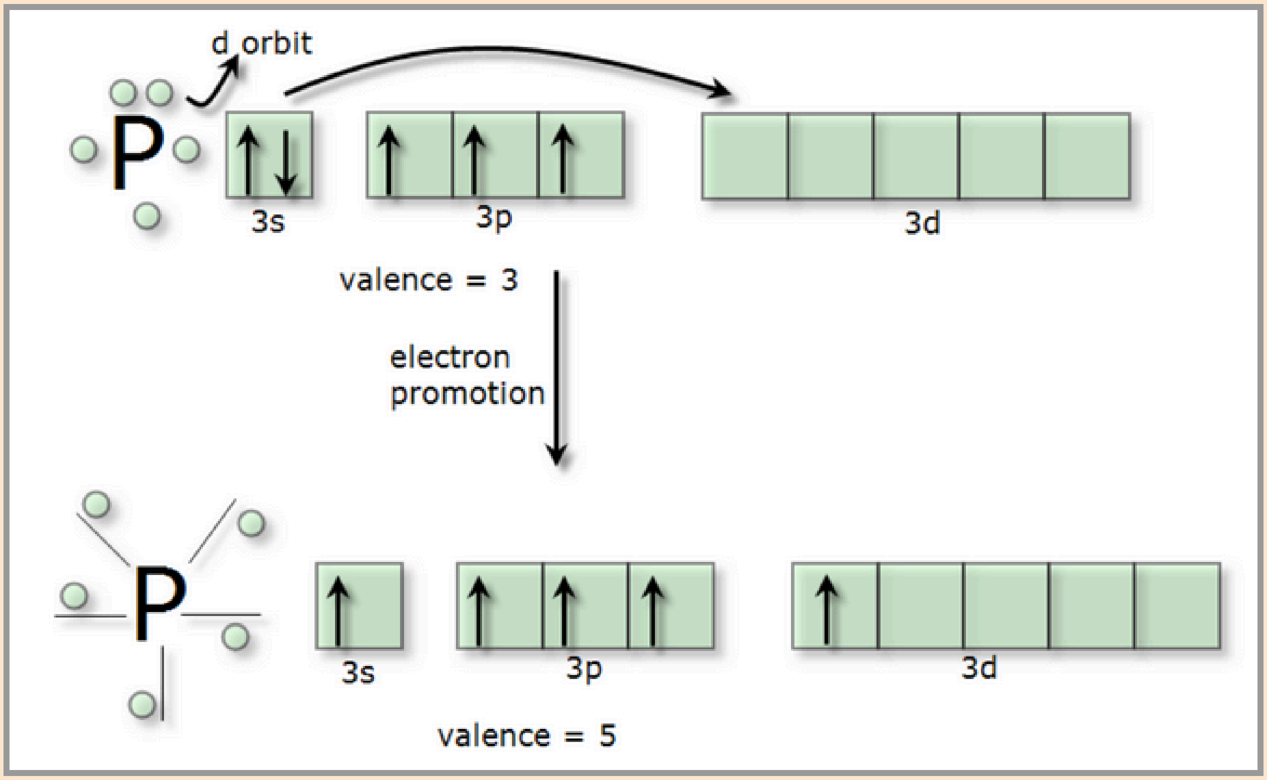


When more than two electrons are shared between two atoms, we have double (4 electrons shared) or triple bonds (six electrons shared):



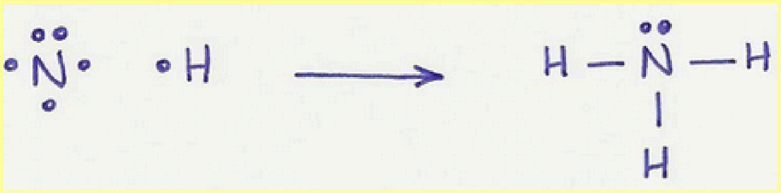
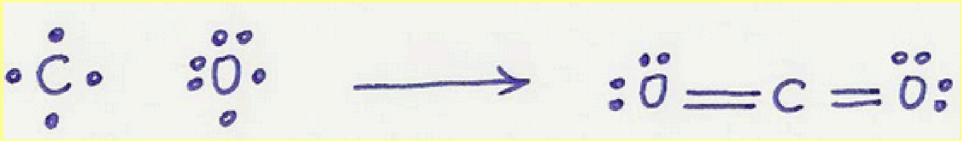
ELECTRON PROMOTION

In order to have more electrons unpaired (to form covalent bonds) an atom can undergo a electron promotion: one or more electrons can jump between orbits at the same level.



EXERCISES AND HOMEWORK

Covalent Bonds - Solutions to Exercises

EXERCISE: Draw the following molecules, using the Lewis notation	
NH_3	
CO_2	

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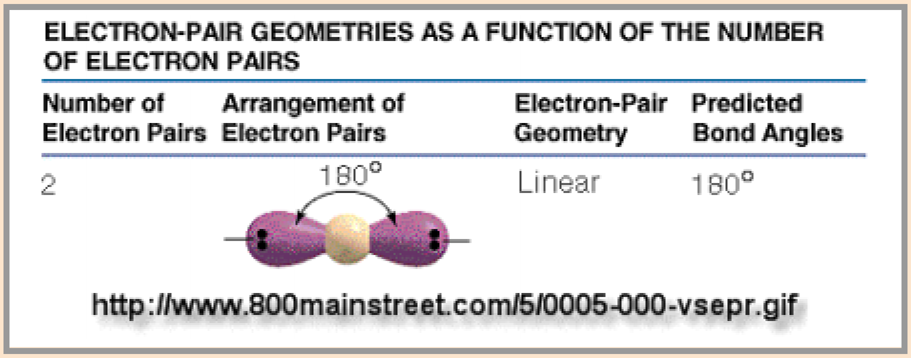
Session 03. Molecular shape: Introduction and molecules composed of three atoms
[Molecular Shape] [Image: molecular shape]

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)


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

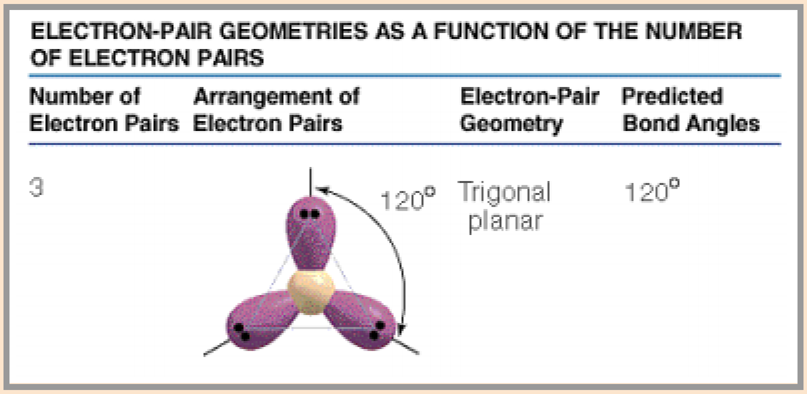
Number of Electron Pairs	Arrangement of Electron Pairs	Electron-Pair Geometry	Predicted Bond Angles
2	180°	Linear	180°

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).

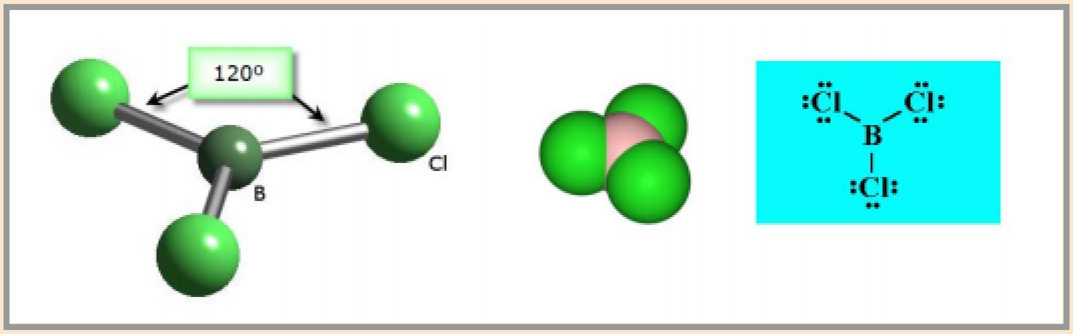
MOLECULAR SHAPES WITH THREE ELECTRON GROUPS (TRIGONAL PLANAR ARRANGEMENT)
Three electron groups around the central atom repel each other to the corners of an equilateral triangle, which gives the trigonal planar arrangement.



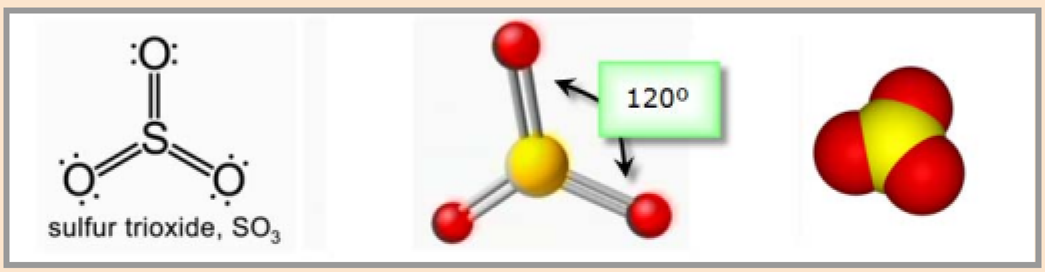
ELECTRON-PAIR GEOMETRIES AS A FUNCTION OF THE NUMBER OF ELECTRON PAIRS

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

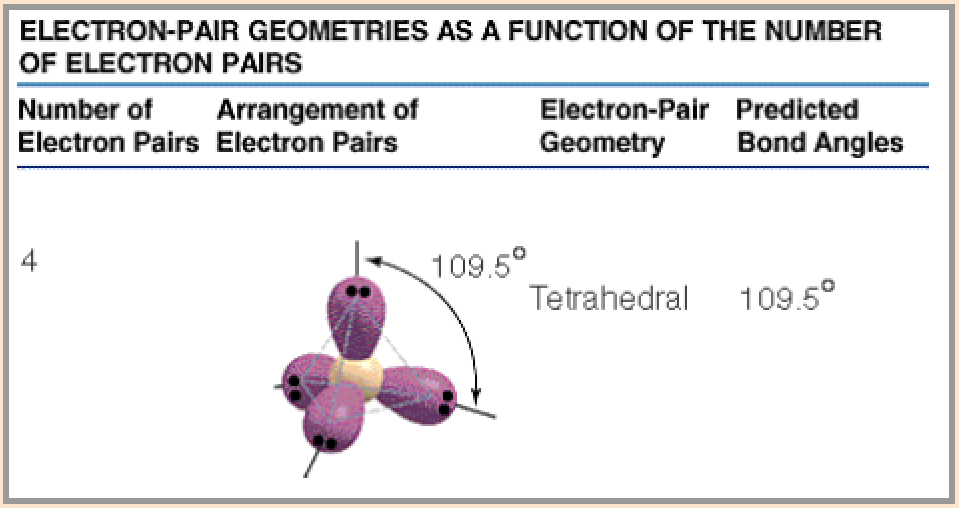
When the three electron groups are bonding groups, the molecular shape is also trigonal planar (AX3; A=Central atom, X=Surrounding atom). Boron trichloride is a trigonal planar molecule:



Sulphur trioxide molecule has the same shape:



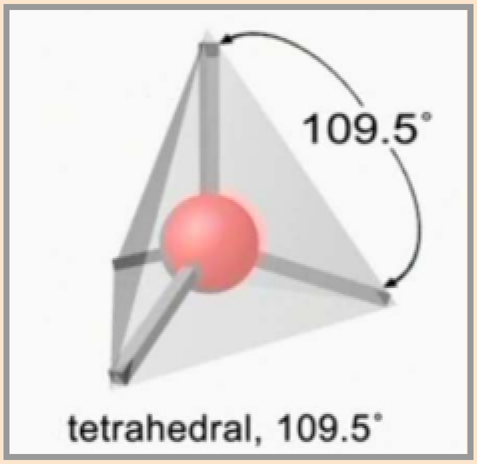
MOLECULAR SHAPES WITH FOUR ELECTRON GROUPS (TETRAHEDRAL ARRANGEMENT)
The shapes described so far have all been easy to depict in two dimensions, but four electron groups must use three dimensions to achieve maximal separation.



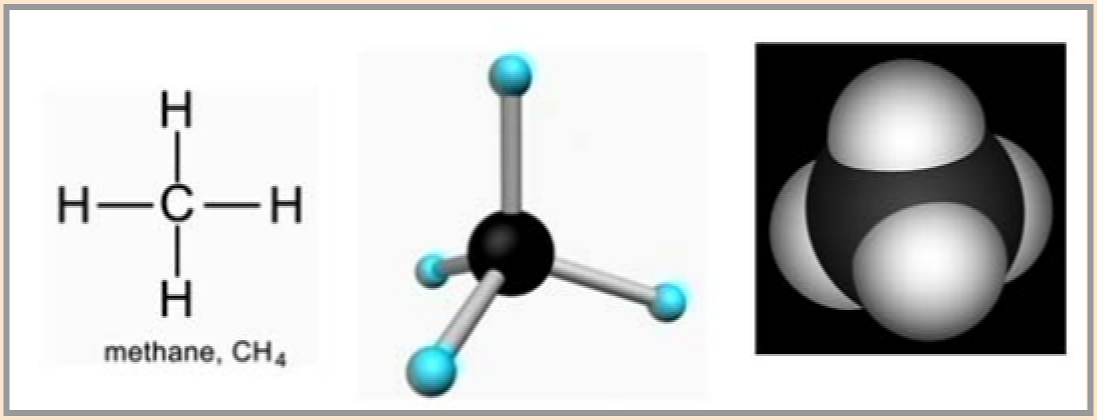
ELECTRON-PAIR GEOMETRIES AS A FUNCTION OF THE NUMBER OF ELECTRON PAIRS

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

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

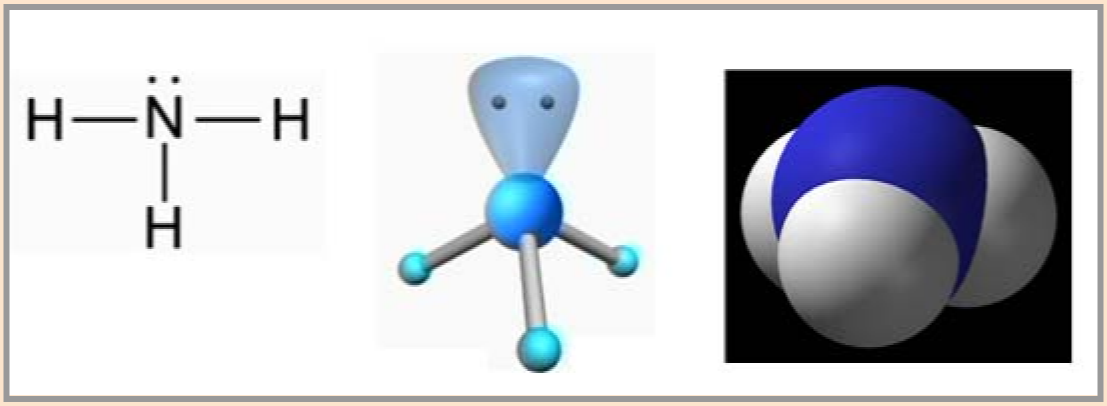


When all four electron groups are bonding groups, as in the case of methane, the molecular shape is also tetrahedral (AX_4). Methane has a bond angle of 109.5º:

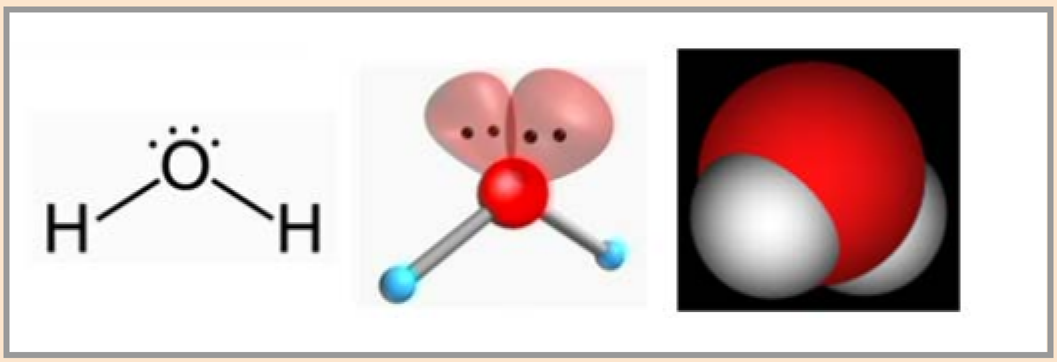


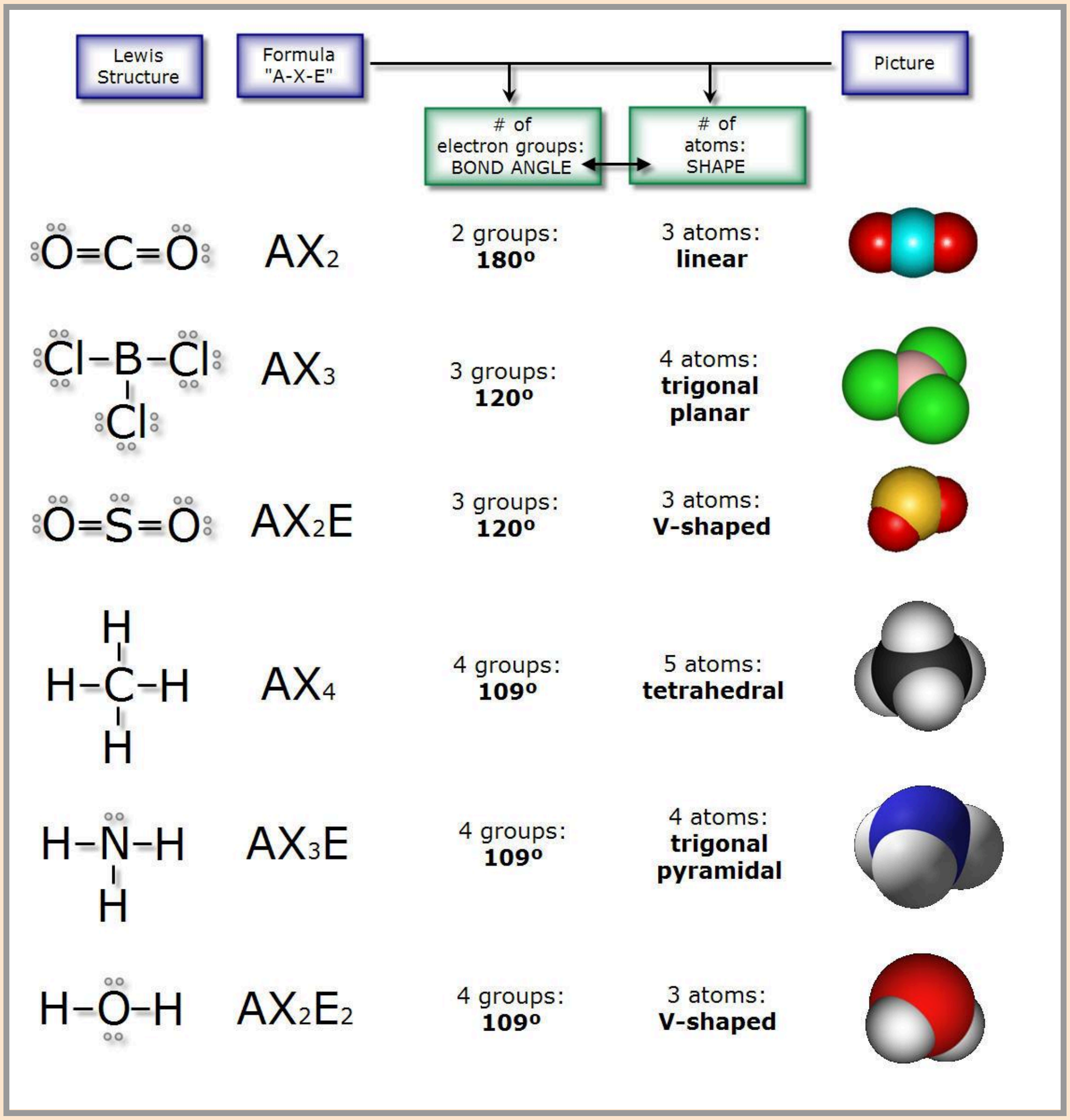
When one of the four electron groups in the tetrahedral arrangement is a lone pair, the molecular shape is that of a trigonal pyramid (AX_3E; A=central atom, X=surrounding atom, E=lone pair). In ammonia (NH_3) the lone pair forces the N-H bonding pairs closer, and the

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.





Lewis Structure
Formula "A-X-E"
# of electron groups: BOND ANGLE
# of atoms: SHAPE
Picture
AX_2
2 groups: 180º
3 atoms: linear
AX_3
3 groups: 120º
4 atoms: trigonal planar
AX_2E
3 groups: 120º
3 atoms: V-shaped
AX_4
4 groups: 109º
5 atoms: tetrahedral
AX_3E
4 groups: 109º
4 atoms: trigonal pyramidal
AX_2E_2
4 groups: 109º
3 atoms: V-shaped

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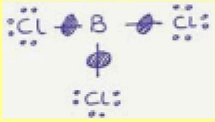
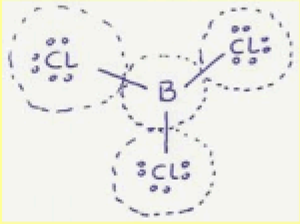
Session 04. Molecular shape and Exercises [Exercises and Solutions]

Molecular Shape: EXERCISES					
Form.	Lewis and electron groups	A-X-E	Electron groups	Atoms SHAPE	Molecule
BCl_3		AX_3	3 groups 120º	4 atoms TRIGONAL PLANAR	
CH_4					
$CHCl_3$					

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Session 05. Polarity [Topic: Polarity of Molecules]

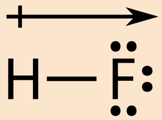
ELECTRONEGATIVITY AND POLARITY OF A BOND [Molecular_Polarity]

When two atoms form a covalent bond they share electrons. This sharing can be equal [non-polar covalent bond, where the sharing is 50 % for each atom] or non-equal [polar covalent bond, where one of the atoms share more than 50% and the other less than 50%]. A 50% sharing means that 50% of the time the shared electrons will be closer to that atom.

The type of sharing is given by the difference in electronegativity between both atoms. Let's take the case of HF, where fluorine (F) has a value of electronegativity of 4 and hydrogen (H) is 2.1. This means that fluorine attracts with higher strength the shared electrons. The difference in electronegativity is 1.9 in favor of fluorine. As a consequence, fluorine will take more than 50% the shared electrons.

This covalent bond is called polar, because the molecule of HF will have two electric poles: fluorine will be the negative electric pole of the molecule [it takes shared electrons more of the time and electrons are negatively charged] and hydrogen will be the positive end of the molecule.

The polarity of a bond can be represented as a polarity arrow and the direction of that arrow describes the displacement of shared electrons towards the more electronegative element:

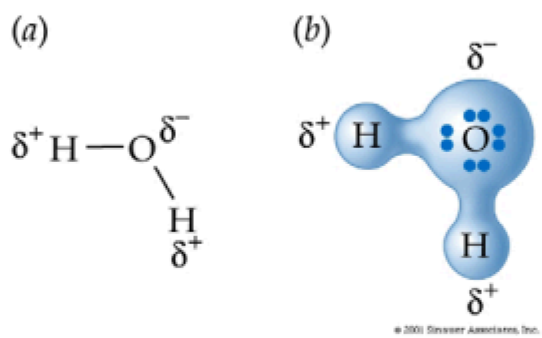


In this case the electronegativity of fluorine is higher and shared electrons are displaced towards fluorine.

These polarity arrows are useful because the polarity of a whole molecule can be determined by the vectorial addition of those arrows.

Electronegativity and Bond Polarity

Electronegativity (EN) is the relative ability of a bonded atom to attract the shared electrons.

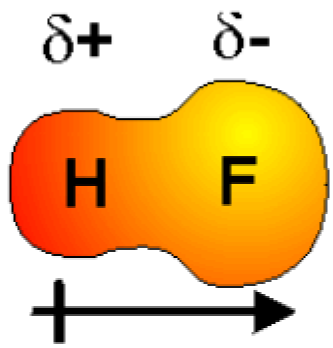


When bonded atoms with different electronegativities form a bond, the bonding pair is shared **unequally**, so the bond has **partially negative** and **positive poles**.

This type of bond is called a polar covalent bond and is depicted by a polar arrow (⟼) pointing toward the negative pole, or by δ^+ and δ^- symbols, where the lower case delta, δ, represents a partial charge.

In the H-H and F-F bonds the atoms are identical, so the bonding pair is **shared equally** and the bond is called a **nonpolar covalent bond**.

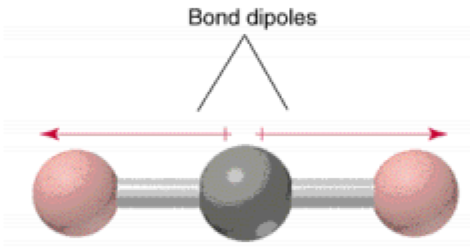
Thus, by knowing the EN values of the atoms in a bond, you can determine the direction of the bond polarity.



http://www.uoregon.edu/~ch111/images/hfpolar.gif

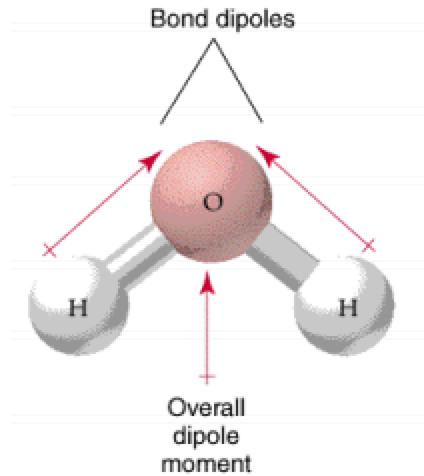
POLARITY OF MOLECULES: EXAMPLES[Molecular Polarity] [Summary]

In order to be a polar molecule, bonds have to be polar: if each bond is non-polar, the whole molecule will be non-polar. In the case of polar bonds, the overall polarity of the molecule could be polar (different from zero) or non-polar (net polarity equal to zero).



Each C=O bond is quite polar. However, CO_2 is linear , so its bonds point 180 ° from each other. As a result, these identical bond polarities are counterbalanced and give the molecule no net polarity.

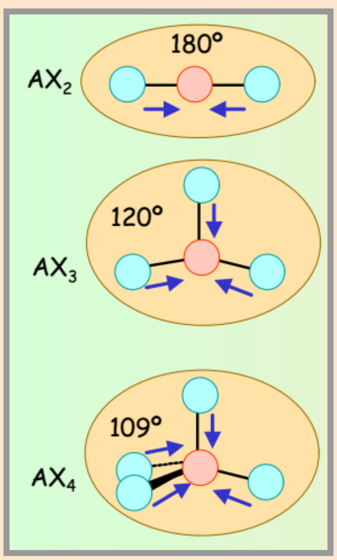
In the case of water the bond polarities are not counterbalanced because the water molecule is V shaped.



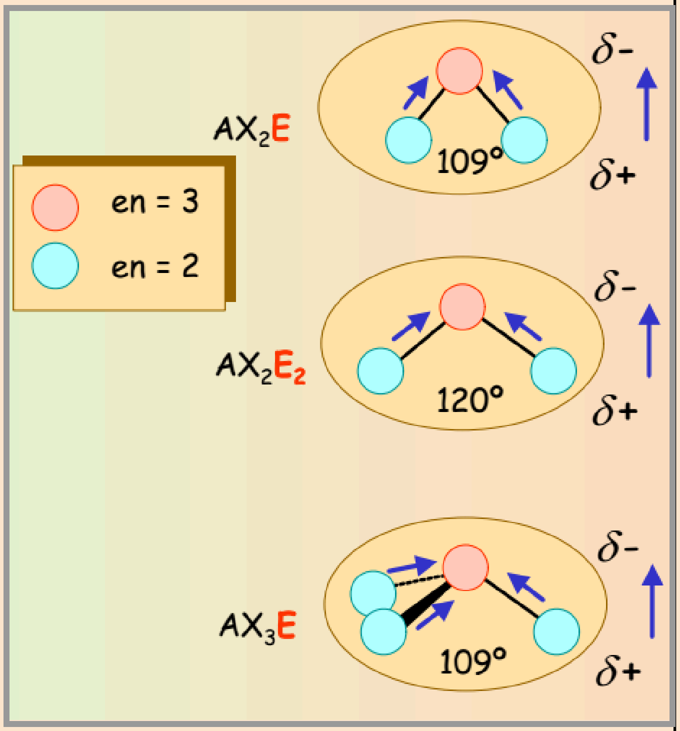
Thus, the O end of the molecule is more negative than the other end.

As a general rule, we can apply the following criteria in order to decide if a molecule is polar or nonpolar:

When polarity arrows are identical, net polarity will be null [non-polar molecule] in the following cases:

	(1) Two arrows at an angle of 180º (linear molecules). The directions of both arrows have to be opposite (2) Three arrows at an angle of 120º (trigonal planar molecules) (3) Four arrows at an angle of 109º egiten (tetrahedral molecules)

In the following cases the net polarity will be different from zero [polar molecules]:



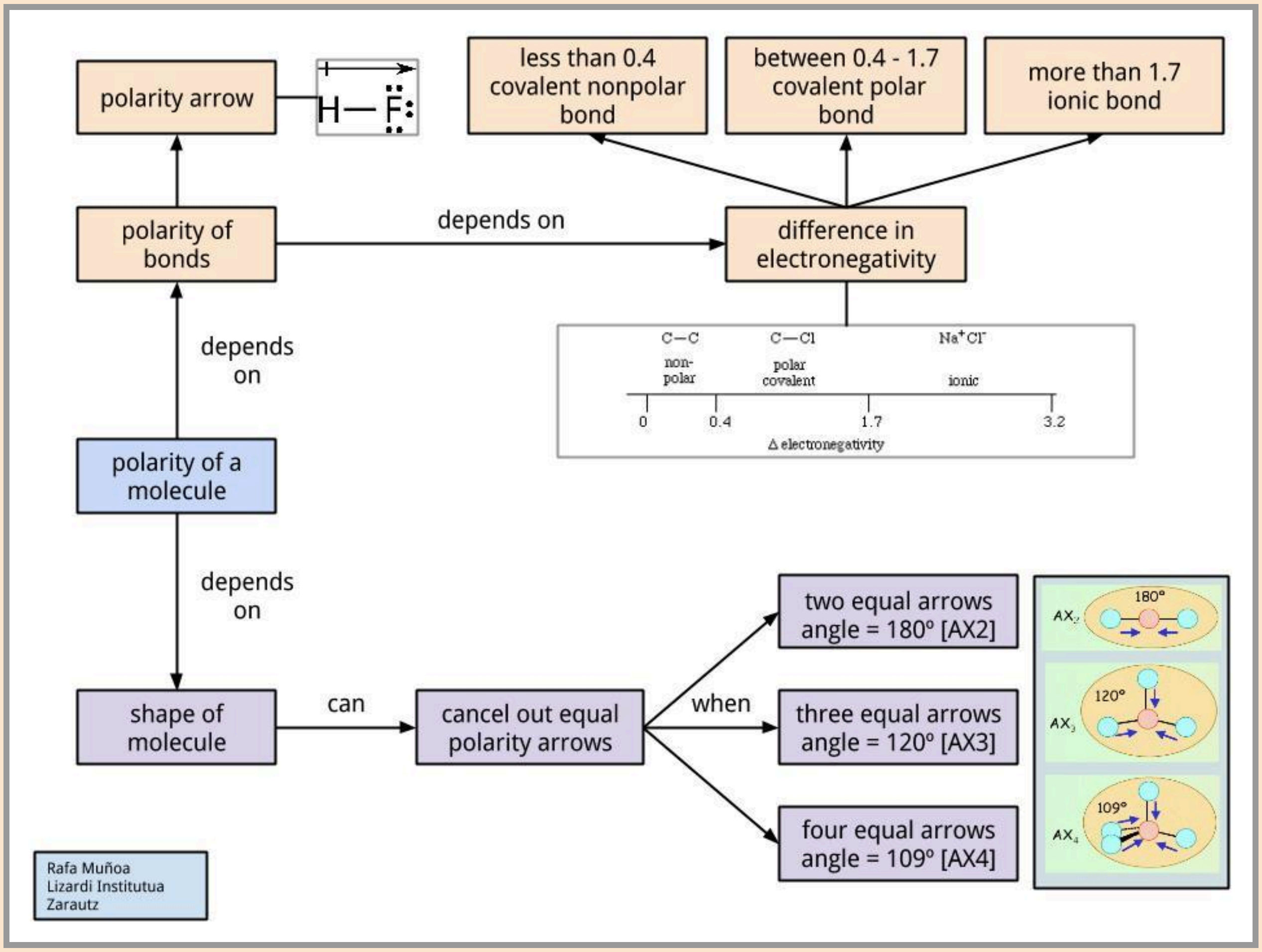
These molecules have net polarity different from zero.

The blue net arrow is in the direction of the negative end of molecules.

If we split those molecules in two parts, one half will be more positive and the other more negative.

We can say that in the case of identical polarity arrows the net value will be zero when there are not non-bonding electron pairs (without E groups) and net polarity will be different from zero when there are non-bonding pairs (there are E groups).

SUMMARY



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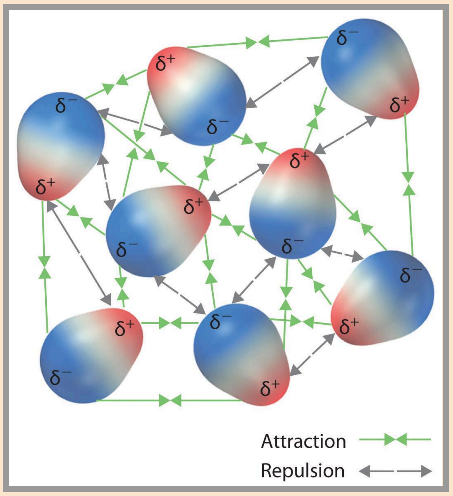
Session 06. Intermolecular Forces [Topic: [Intermolecular Forces]]

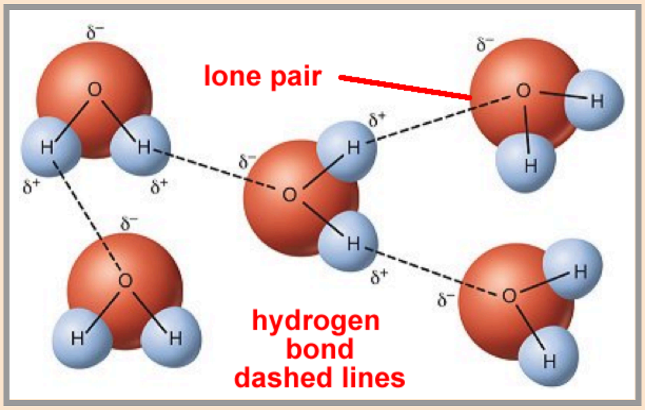
INTERMOLECULAR FORCES [[Intermolecular forces CMap]]
Intermolecular forces are electrostatic forces that depend on polarity of molecules: opposite partial charges will attract each other

Intermolecular forces among polar molecules are called dipole-dipole forces:



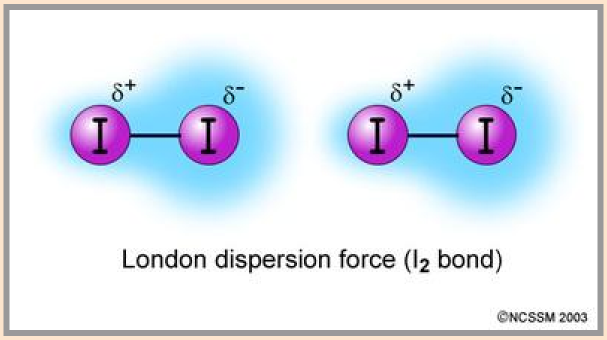
Here we can see how molecules adopt the orientation that maximizes attraction forces and minimize repulsion forces.

Polar molecules can form a strong intermolecular force called hydrogen bonds if they meet two conditions: (1) the negative end of molecule includes a highly electronegative element (F fluorine, O oxygen or N nitrogen) and (2) the positive end of molecule contains a hydrogen that is bonded to one of the mentioned highly electronegative element.



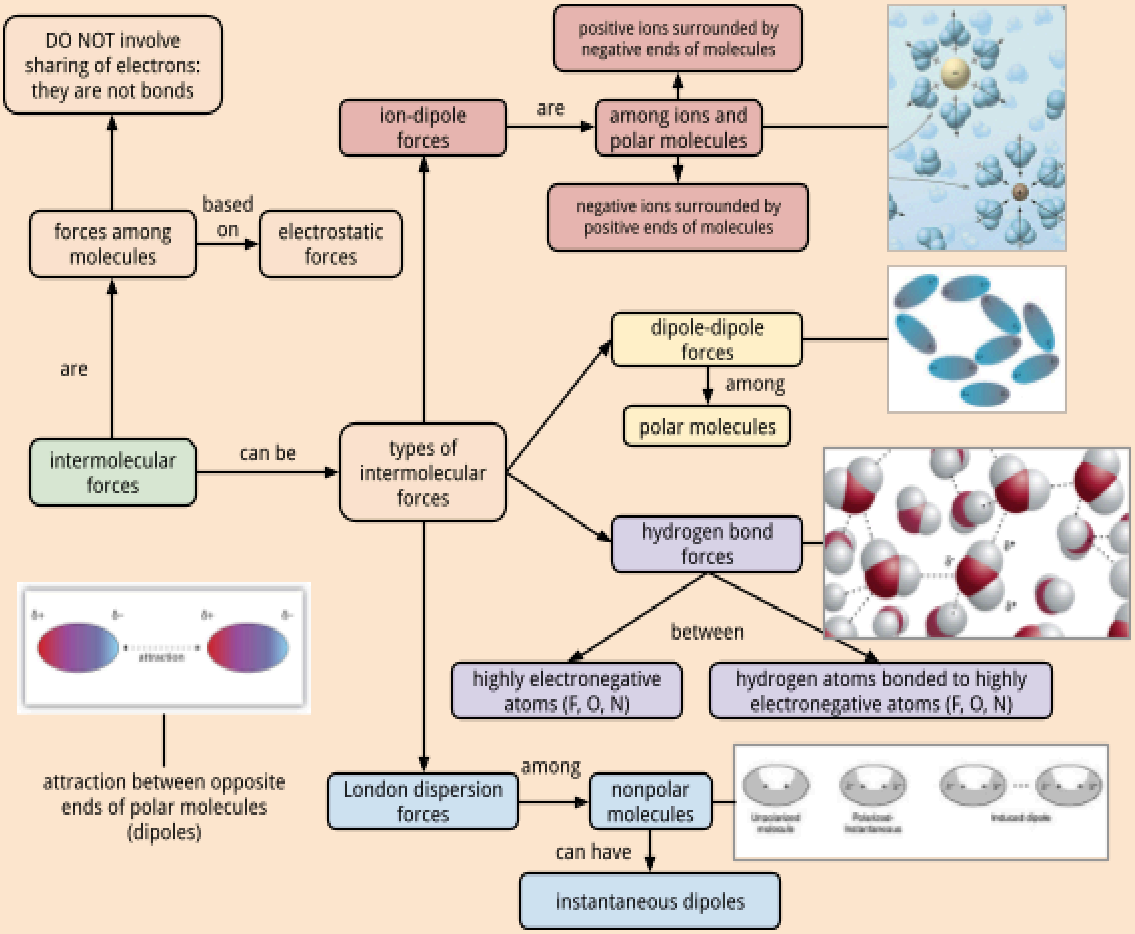
This hydrogen bonds happen in molecules such as water, ammonia, and alcohols.

Intermolecular forces can happen among nonpolar molecules; this type of force is called London dispersion forces and the reason is that even though molecules are nonpolar, they form instantaneous dipoles (electrons are moving) and thus, instantaneous attraction forces appear.



Iodine molecule forms instantaneous dipoles (because of motion of electrons) and London dispersion forces appear.

A summary of intermolecular forces:



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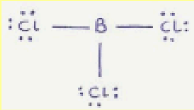
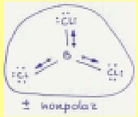
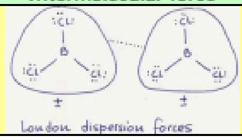
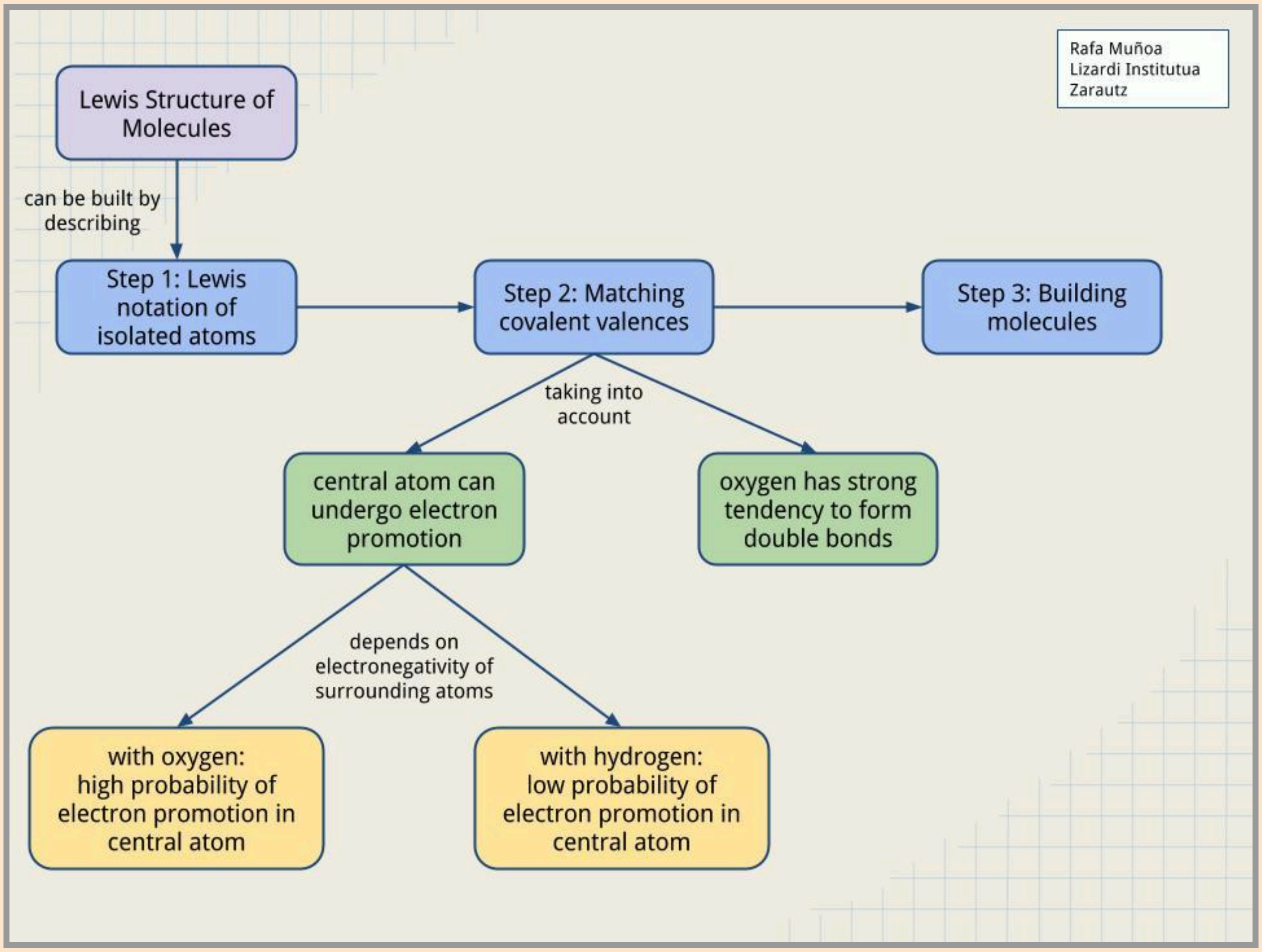
Session 07. Integrated Exercise [Integrated_Exercise and Integrated_Exercise_Sol]

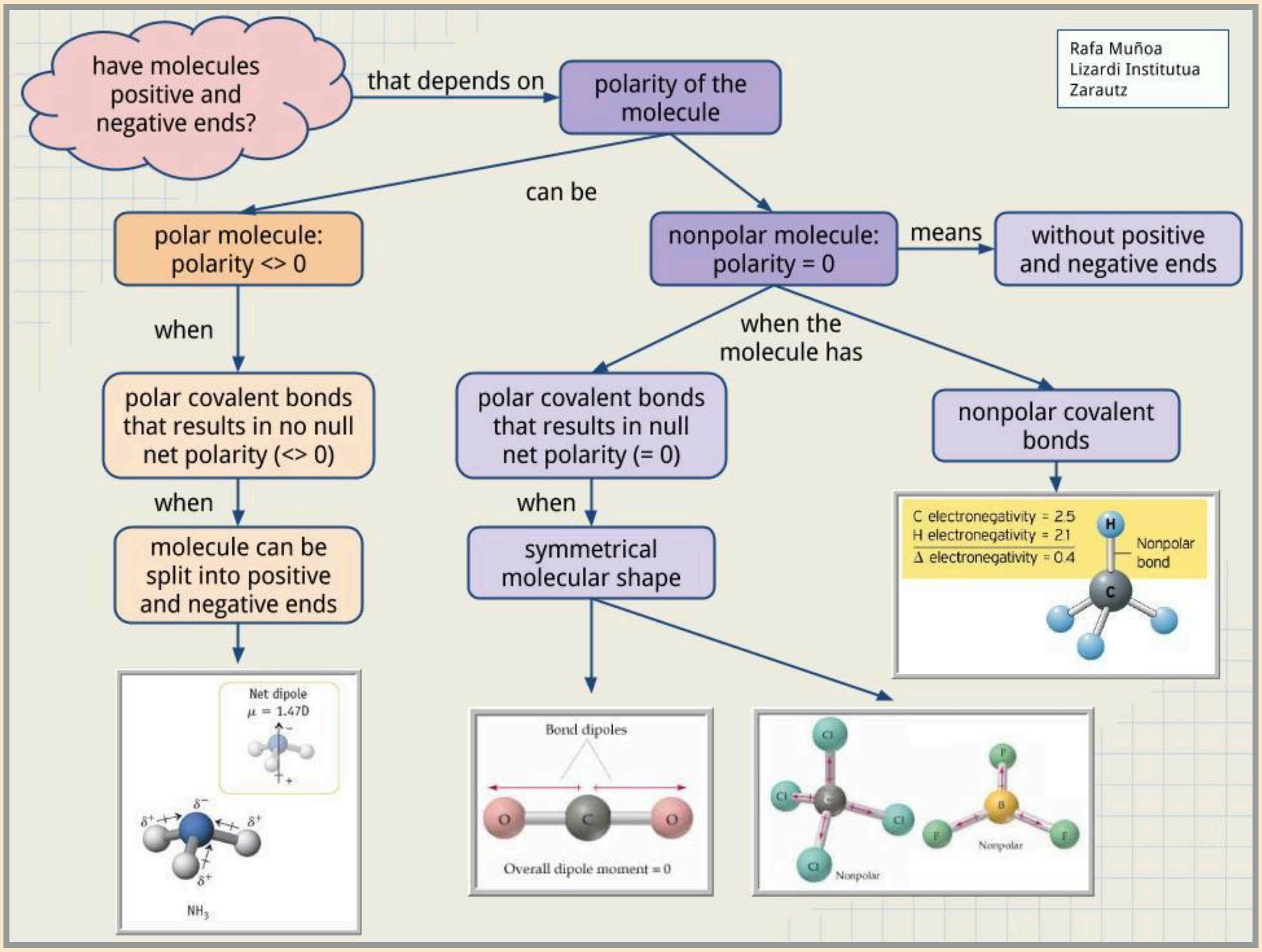
Fill in the table

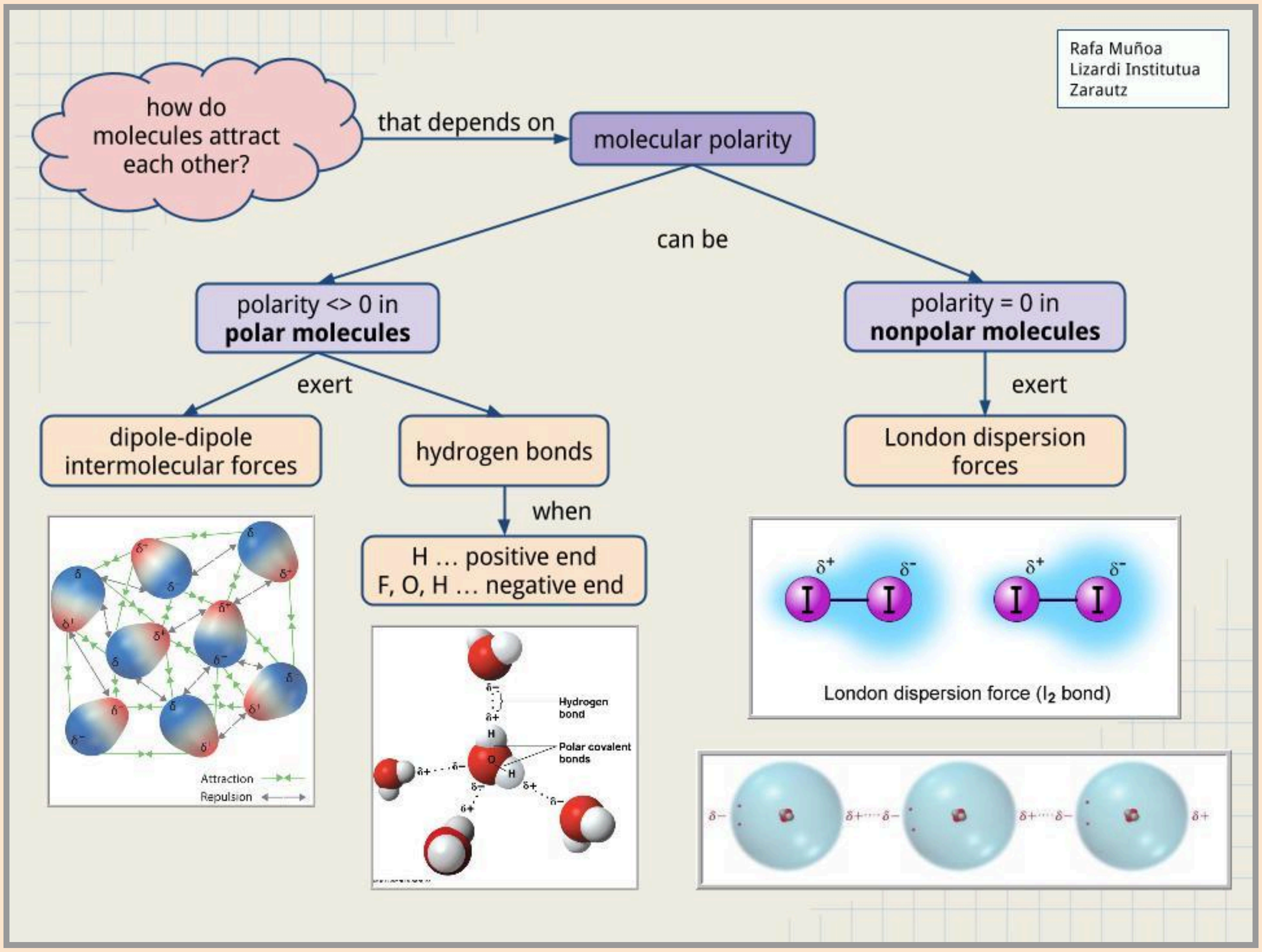
EXERCISE. Complete the information below:				
Formula	**Lewis Structure**	**Shape**	**Polarity**	**Intermolecular force**
BCl_3				
CO_2				
CH_4				
CH_3Cl				
NH_3				

An Integrated Exercise
Chemical Bonding
1
Rafa Muñoa
Lizardi Institutua

Questions we need to ask ourselves:


Rafa Muñoa
Lizardi Institutua
Zarautz
Lewis Structure of Molecules
can be built by describing
Step 1: Lewis notation of isolated atoms
Step 2: Matching covalent valences
Step 3: Building molecules
taking into account
central atom can undergo electron promotion
oxygen has strong tendency to form double bonds
depends on electronegativity of surrounding atoms
with oxygen: high probability of electron promotion in central atom
with hydrogen: low probability of electron promotion in central atom


Rafa Muñoa
Lizardi Institutua
Zarautz
have molecules positive and negative ends?
that depends on
polarity of the molecule
can be
polar molecule: polarity <> 0
nonpolar molecule: polarity = 0
means
without positive and negative ends
when
when the molecule has
polar covalent bonds that results in no null net polarity (<> 0)
polar covalent bonds that results in null net polarity (= 0)
nonpolar covalent bonds
when
when
molecule can be split into positive and negative ends
symmetrical molecular shape
C electronegativity = 2.5
H electronegativity = 2.1
Δ electronegativity = 0.4
Nonpolar bond
Net dipole
μ = 1.47D
NH3
Bond dipoles
Overall dipole moment = 0
Nonpolar
Nonpolar


Rafa Muñoa
Lizardi Institutua
Zarautz
how do molecules attract each other?
that depends on
molecular polarity
can be
polarity <> 0 in
polar molecules
polarity = 0 in
nonpolar molecules
exert
exert
dipole-dipole intermolecular forces
hydrogen bonds
London dispersion forces
when
H … positive end
F, O, H … negative end
Attraction
Repulsion
Hydrogen bond
Polar covalent bonds
London dispersion force (I_2 bond)

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Session 08. Properties of substances [Physical properties of substances] [Melting and boiling points of substances] [Properties of ionic bonds] [Physical properties of metals]

Physical Properties of Substances							
Type of substance	Example		Physical State (at room T)	Melting Point	Mechanical Properties	Electrical Properties	Solubility in water (Y/N)
IONIC (Ionic Network)	-Metallic oxides -Hydroxides -Binary salts -Oxysalts	-MgO -$NaOH$ -Na_2S -$CaCO_3$	Solid	High	Brittle	Insulator Conductor when melt or dissolved in water	Yes
COVALENT MOLECULAR (Molecules)	-Nonmetallic oxides -Binary acids -Oxoacids	-CO_2 -HCl -H_2SO_4	Any state Solid / Liquid / Gas	Low	Soft	Insulator	Polar molecules only
COVALENT NETWORK STRUCTURES (Covalent Network)	-Diamond -Quartz		Solid	High	Hard	Insulator	No
METALLIC (Metallic Network)	-Metallic elements	-Fe	Solid	High	Malleable Ductile	Conductor	No

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