

CHEMICAL BONDING I

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Purpose

The purpose of this experiment is to determine molecular geometries of simple molecules, and to use molecular geometries and electronegativity data to determine whether molecules are polar or nonpolar.

Theory

The molecular geometry of a molecule is the shape or the three-dimensional manner in which the atoms project into space. The shape of a molecule is important because it affects the polarity of the molecule. The polarity of a molecule affects physical properties such as solubility, melting point, and boiling point.

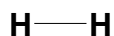
In order to predict the molecular geometry of a molecule, one must consider the number of bonds and the number of nonbonding electrons around the central atom. The arrangement of bonds and nonbonding electrons, and whether the bonds are polar or nonpolar, will determine whether the molecule is polar or nonpolar. Whether a bond is polar or nonpolar is determined by the electronegativity difference between the atoms making up the bond. The electronegativity values for the elements are shown in the periodic table on the following page. Notice that electronegativity values generally increases from left to right across each period and decreases from top to bottom in the groups in the table.

I A	II A											III A	IV A	V A	VI A	VII A	VIII A
2.1 H																	
1.0 Li	1.5 Be											2.0 B	2.5 C	3.0 N	3.5 O	4.0 F	
0.9 Na	1.2 Mg	III B	IV B	V B	VI B	VII B	VIII B		IB	IIB		1.5 Al	1.8 Si	2.1 P	2.5 S	3.0 Cl	
0.8 K	1.0 Ca	1.3 Sc	1.5 Ti	1.6 V	1.6 Cr	1.5 Mn	1.8 Fe	1.8 Co	1.8 Ni	1.9 Cu	1.6 Zn	1.6 Ga	1.8 Ge	2.0 As	2.4 Se	2.8 Br	
0.8 Rb	1.0 Sr	1.2 Y	1.4 Zr	1.6 Nb	1.8 Mo	1.9 Tc	2.2 Ru	2.2 Rh	2.2 Pd	1.9 Ag	1.7 Cd	1.7 In	1.8 Sn	1.9 Sb	2.1 Te	2.5 I	
0.7 Cs	0.9 Ba	1.1 La	1.3 Hf	1.5 Ta	1.7 W	1.9 Re	2.2 Os	2.2 Ir	2.2 Pt	2.4 Au	1.9 Hg	1.8 Tl	1.9 Pb	1.9 Bi	2.0 Po	2.2 At	
0.7 Fr	0.9 Ra	1.1 Ac															

The electrons in a bond are shared equally between the atoms when the atoms have the same electronegativity values. In such a situation the electronegativity difference between the atoms is zero and the bond that forms is a **nonpolar covalent bond**. When the electronegativity difference between two atoms is small the bond that forms is a **polar covalent bond**, and if the electronegativity difference is large the resulting bond is likely to be **ionic**. In general an electronegativity difference between zero and two results in a polar covalent bond. An ionic bond results when the difference is larger than two.

You can predict the polarity of bonds using electronegativity data. However, it is also important to be able to predict the polarity of molecules. The terms “polar” and “nonpolar” when used to describe molecules refers to the distribution of charge in a molecule. In a polar molecule the charge is unequally distributed. In these situations the molecule has one positive end and one negative end. In a nonpolar molecule the charge is equally distributed and the molecule does not have positive and negative ends.

First, let's consider a hydrogen gas molecule. Both hydrogen atoms in this molecule have the same electronegativity value. As a result both atoms share the two electrons in the covalent bond equally. This results in an equal distribution of charge. As a result hydrogen gas molecules are **nonpolar**.



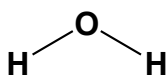
No positive or negative charges

Now let's consider beryllium chloride. Beryllium chloride molecules have a linear geometry with the beryllium atom in the center. The two chlorine atoms have a higher electronegativity than the beryllium atom. The electrons in the two bonds will not be shared equally because of this. The electrons will reside closer to the chlorine atoms because of the higher electronegativity of chlorine. Since the molecule is linear the overall distribution of charge is symmetrical and the molecule is **nonpolar** even though the bonds that make up the molecule are polar. The molecule does not have one positive end and one negative end. The negative and positive charges cancel each other out. The figure below shows the charge distribution in the molecule. The partial negative charges (designated with the symbol δ^-) result from the higher electronegativity of the chlorine atoms and the partial positive charge (δ^+) results from the lower electronegativity of the beryllium atom.



δ^- δ^+ δ^-

Now let's consider water molecules. Water molecules are non-linear or bent. The two hydrogen atoms have a lower electronegativity value than the oxygen atom. As a result the electrons in the two bonds will reside closer to the oxygen atom. Since the water molecule is bent the charge distribution is not symmetrical. The molecule has a negative end and a positive end. The negative end is at the top of the molecule and the positive end is at the bottom of the molecule. (See the picture below.) This unsymmetrical distribution of charge results in a **polar** molecule. As you can see, you must know the correct molecular geometry of a molecule before you can determine the polarity of the molecule. As in the figure shown above, the partial positive and negative charges in the molecule are caused by the difference in electronegativity of the atoms.



δ^-
 δ^+ δ^+

In this experiment you will view a number of molecular models to visualize the three-dimensional shapes of some molecules. These molecules will contain single bonds, double bonds and triple bonds.

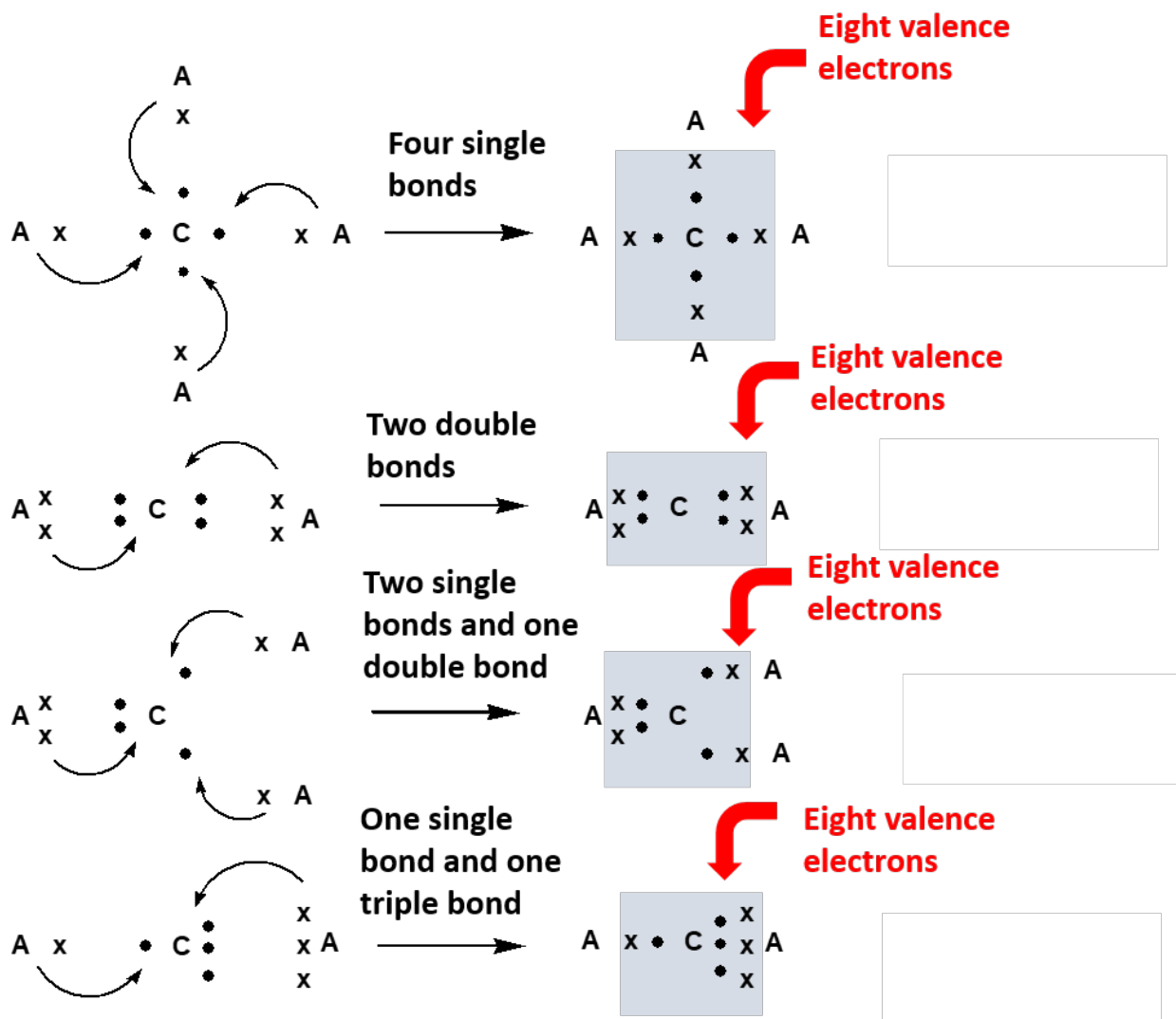
- A single bond is a covalent bond in which a single pair of electrons is shared between two atoms.
- A double bond is a covalent bond in which two pairs of electrons are shared between two atoms.
- A triple bond is a covalent bond in which three pairs of electrons are shared between two atoms.

The number and type of bonds that an atom forms depends on the number of electrons it needs to satisfy the octet rule. For example, a carbon atom has four valence electrons and therefore needs to share four more with other atoms to fulfill the octet rule when forming covalent bonds. This can be accomplished by forming:

- Four single bonds
- Two double bonds
- One double bond and two single bonds
- One triple bond and one single bond

In each case the carbon atom has eight electrons in its outer shell after bonding. The diagram below shows the four different bonding combinations that help carbon atoms obey the octet rule. The "A" refers to the atom bonded to the carbon atom, the "x"s refer to electrons on "A" and the dots refer to electrons on carbon.

- Notice that in all cases carbon has **zero** nonbonding electrons.
- Also notice that in all cases the carbon atom has **eight** valence electrons and is satisfying the octet rule.



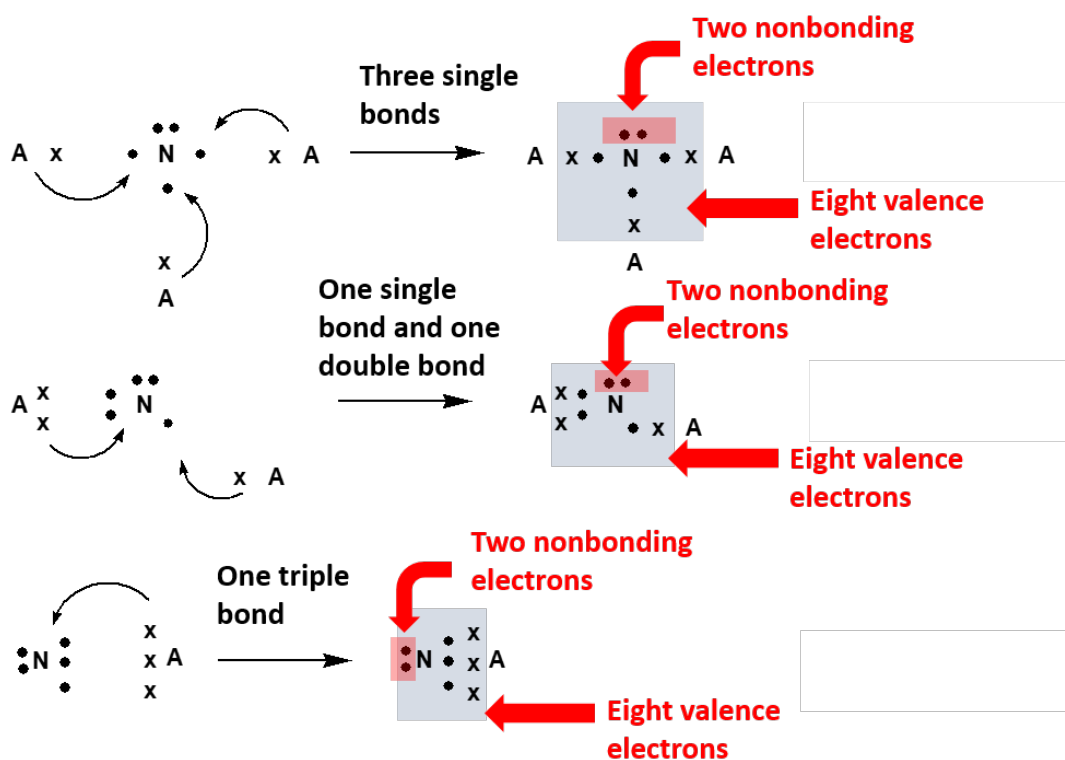
In each case the bonds are symmetrically spaced around the carbon atom so that all bonds are as far from each other as possible. Also notice that each carbon atom is sharing eight electrons. The number of "x"s and dots around each carbon atom adds to eight.

Similar analyses can be performed with other atoms. For example, nitrogen has five valence electrons and therefore needs three more electrons to fulfill the octet rule. This can be accomplished by forming the following covalent bonds.

- Three single bonds
- One double bond and one single bond
- One triple bond

The diagram below shows the three bonding combinations for nitrogen. In the diagram the "A" refers to the atom bonded to the nitrogen atom, the "x"s refer to electrons on "A" and the dots refer to electrons on nitrogen.

- Notice that in all cases nitrogen has **two** nonbonding electrons.
- Also notice that in all cases the nitrogen atom has **eight** valence electrons and is satisfying the octet rule.



In determining the shape of the molecule the bonding and nonbonding electrons will be as far apart from each other as possible just as they were in the molecules containing carbon atoms.

In summary, the number of valence electrons that an atom has will determine the number and type of bonds an atom needs to fulfill the octet rule. The arrangement of bonding and nonbonding electrons determines the shape or geometry of the molecule which can then be used to make judgments about the polarity of the molecule.

Name _____

Date _____

CHEMICAL BONDING I

Prelaboratory Assignment

1. Define electronegativity.

Electronegativity is the measure of the tendency of an atom to attract a bonding pair of electrons

2. What factors are used to determine whether a molecule will be polar or nonpolar?

The electronegativity difference between the bonding atoms. The greater the difference the more the polarity.

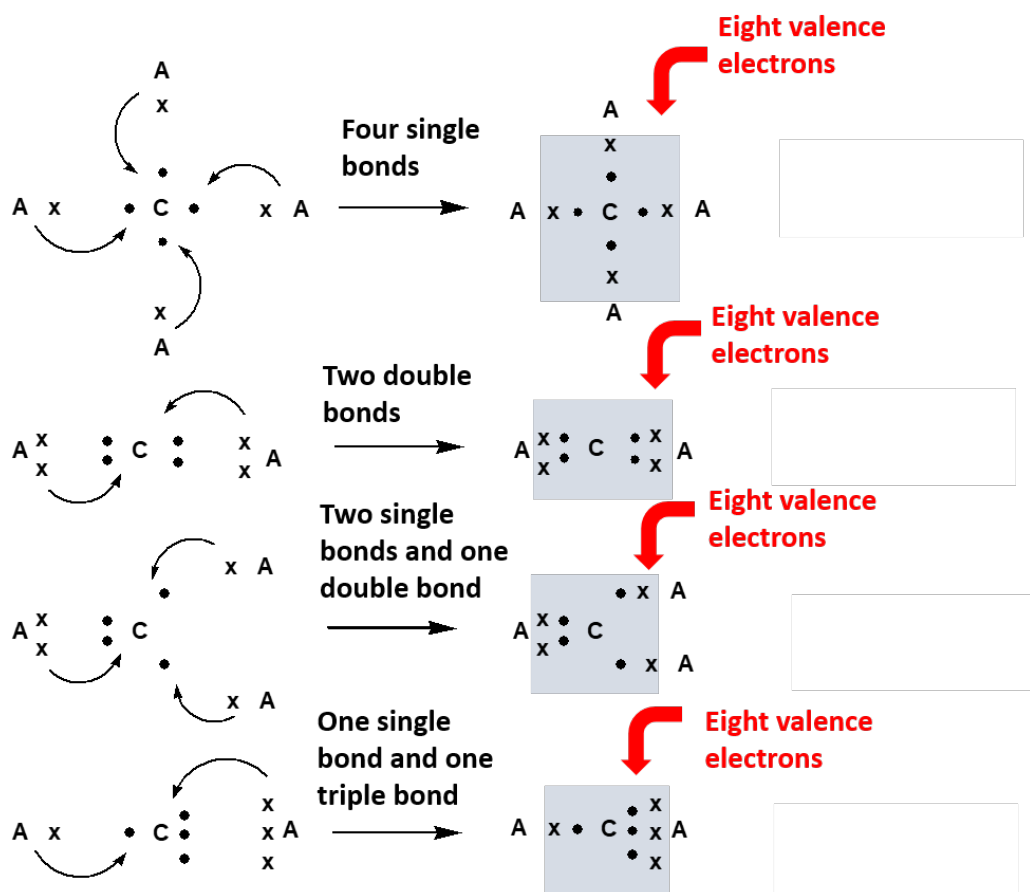
The distance of separation of the charges. Polarity increases with decreasing charge separation distance.

3. What factors are used to determine whether a bond will be polar or nonpolar?

The electronegativity of atoms is normally considered. When the electrons in a bond are shared equally between the atoms when the atoms have the same electronegativity values. The bond formed is covalent as there is no electronegativity difference. When the electronegativity difference between two atoms is small the bond that forms is a polar covalent bond, and if the electronegativity

4. Carbon atoms have four valence electrons. As a result they need four more electrons to obey the octet rule. These electrons can be obtained by sharing electrons with other atoms during covalent bonding. As described in the **Theory** section the combinations of covalent bonds that fulfill the octet rule for carbon in neutral molecules are as follows. See the figure on the following page showing these combinations.

- four single bonds
- two double bonds
- two single bonds and one double bond
- one triple bond and one single bond



The bond combinations for nitrogen were also discussed in the **Theory** section.

a. Now let's think about **oxygen** atoms. How many **valence electrons** does an oxygen atom have?

Six

b. How many **more** electrons does an oxygen atom need to obey the octet rule?

Two

c. What are the combinations of covalent bonds that fulfill the octet rule for oxygen? Keep in mind the following.

- In all bonding combinations an oxygen atom will have **four** nonbonding electrons.

Indicate **Correct** for a correct bonding combination for oxygen. There are only **two** correct bonding combinations for oxygen.

• One single bond Incorrect	• Two single bonds Correct	• Three single bonds Incorrect	• Four single bonds Incorrect
• One double bond Correct	• One double bond and one single bond Incorrect	• Two double bonds Incorrect	• One double bond and three single bonds Incorrect
• One triple bond Incorrect	• One triple bond and one single bond Incorrect	• One triple bond and two single bonds Incorrect	• Two triple bonds Incorrect

5. As described above atoms can form covalent bonds with other atoms to obey the octet rule and to become stable. This means that atoms will form covalent bonds to gain eight valence electrons.

One exception to this is the hydrogen atom. Hydrogen atoms will not form covalent bonds to gain eight valence electrons. Hydrogen atoms only need two valence electrons to become stable. With this in mind, answer the following questions about hydrogen atoms.

a. How many **valence electrons** does a hydrogen atom have?

One

b. How many **more** electrons does a hydrogen atom need to become stable?

One

c. What covalent bond will a hydrogen atom form to become stable? Keep in mind the following.

- In all bonding combinations a hydrogen atom will have **zero** nonbonding electrons.

Indicate **Correct** for a correct bonding combination for hydrogen. There is only **one** correct bonding combination for hydrogen.

• One single bond	• One double bond	• One triple bond
Correct	Incorrect	Incorrect

Name _____

Date _____

CHEMICAL BONDING I

Procedure and Data Sheet

A. Instructions for investigating the bonding patterns and molecular geometries of molecules on the ChemSpider website.

1. Go to <http://www.chemspider.com/>.
2. Type the name of the molecule in the Search ChemSpider field. **Methane** is typed here.

Search ChemSpider

Matches any text strings used to describe a molecule.

methane 

Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID 

3. Hit your Return key. You should see that one result was found. Notice that the **molecular formula** for methane is given.
4. Click on the magnifying glass to see the structure of methane.

Found 1 result

Search term: **methane** (Found by approved synonym)

CH₄



Methane

Molecular Formula	CH ₄
Average mass	16.042 Da
Monoisotopic mass	16.031300 Da
ChemSpider ID	291

↓

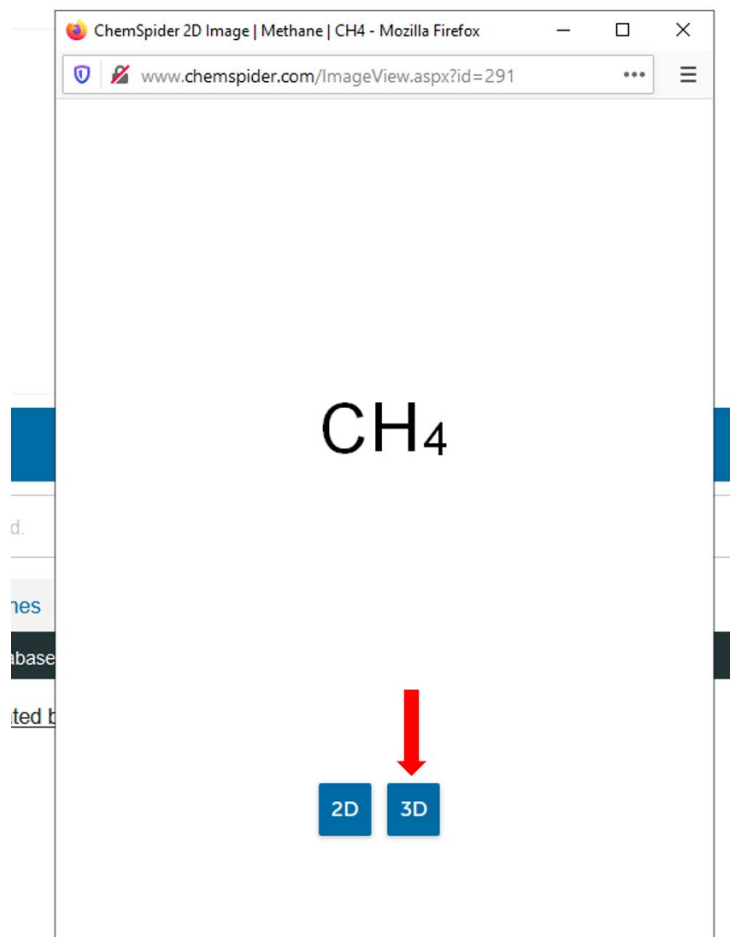
Molecular formula for methane

↓

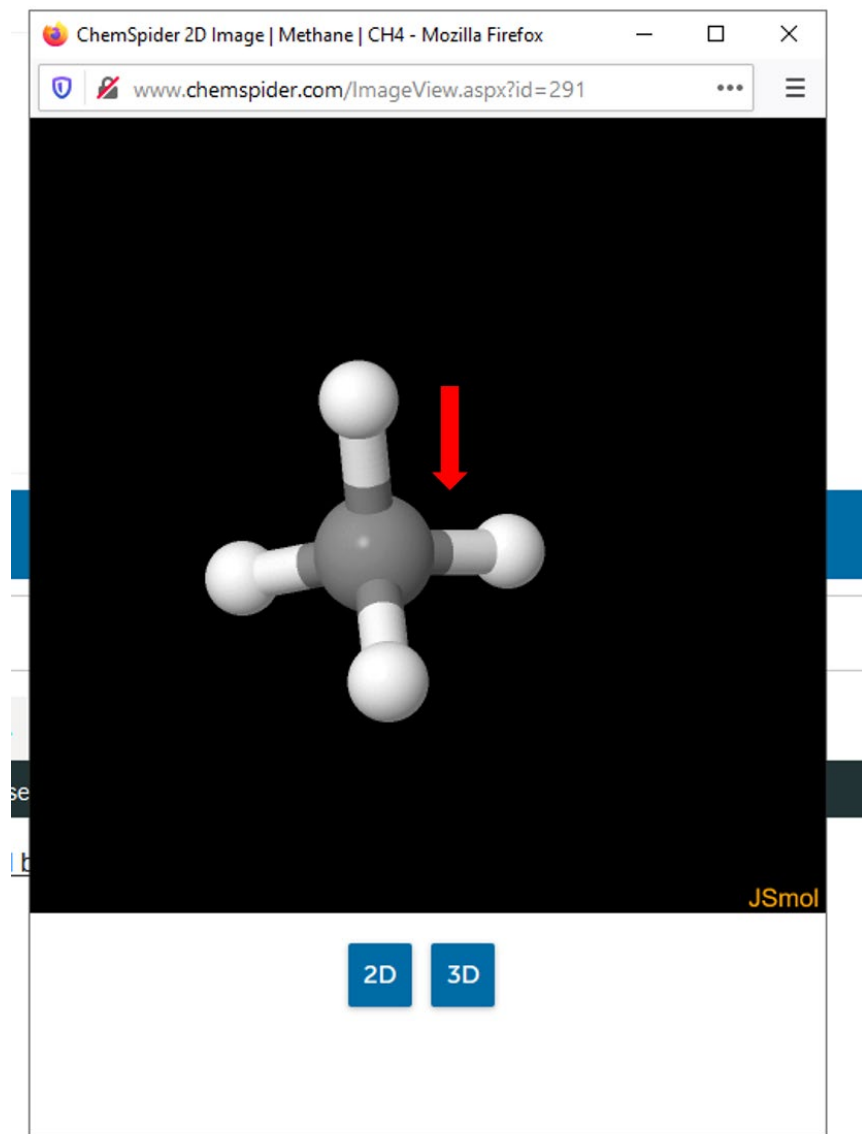
CH₄

More details:

5. A second window should appear. Click on the 3D button.



4. The three-dimensional picture of the molecule should appear. You can rotate the molecule using your cursor.



B. Molecular formulas and molecular polarity

a) Complete the tables below by observing the seven molecules listed below. Follow the instructions for using the ChemSpider website in **Part A** of the **Procedure** to view the molecules. Refer to the discussion in the **Theory** section about molecular polarity to determine whether the following molecules are polar or nonpolar.

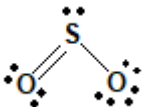
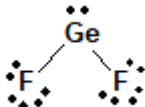
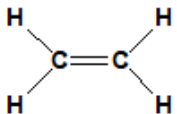
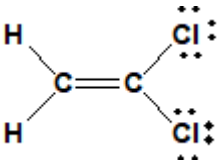
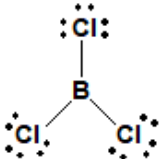
Name	Molecular formula	Is the molecule polar or nonpolar?
Methane	CH ₄	Non-polar
Ammonia	NH ₃	Polar
Hydrogen chloride	HCl	Polar
Dinitrogen	N ₂	Non-polar
Chloroform	CHCl ₃	Non-polar
Formaldehyde	CH ₂ O	Polar
Carbon dioxide	CO ₂	Non-polar

CHEMICAL BONDING I

Questions

1. Complete the table below. Indicate whether the molecules shown below are polar or nonpolar, and indicate the atoms in these molecules that are not obeying the octet rule. **Remember** that the geometries of all these molecules will influence the molecular polarity.

Note: All of these molecules are flat and have the geometries as indicated in the drawings. So for example SO_2 and GeF_2 have bent geometries and are not linear.

Molecule	Indicate whether the molecule is polar or nonpolar by entering POLAR or NONPOLAR.	Indicate which atoms in the molecule are not obeying the octet rule. Enter No if all the atoms in the molecule are obeying the octet rule
	POLAR	NO
	POLAR	Germanium atom
	NONPOLAR	NO
	POLAR	NO
	NONPOLAR	Boron