

Chemistry 500: Chemistry in Modern Living

Topic 3: The Chemistry of Global Warming

Molecular Structures and Moles

Chemistry in Context, 2nd Edition: Chapter 3, Pages 73-110

Chemistry in Context, 3rd Edition: Chapter 3, Pages 93-136

Outline Notes by Dr. Allen D. Hunter, YSU Department of Chemistry, ©2000.

Outline

3A	THE GREENHOUSE EFFECT.....	3
3B	CHANGES IN CO ₂ OVER TIME.....	4
3C	MOLECULES: HOW THEY SHAPE UP.....	6
3D	VIBRATING MOLECULES.....	10
3E	WEIGHING SUBSTANCES.....	13
3F	CALCULATING WITH MOLES.....	16
3G	HUMANS AND CO ₂	18
3H	METHANE AND GLOBAL WARMING.....	20
3I	WHERE DO WE GO FROM HERE: CLIMATE MODELING AND FUTURE CHANGES.....	21

3A The Greenhouse Effect

- What is a **gardening** greenhouse?
 - A heater and a cover (glass or plastic cover)
 - Hand Drawing!

- Earth as a **greenhouse**
 - The **atmosphere** acts as a cover
 - Lets light in but does not let heat out
 - **Graphics from Text: Figure 3.2, the Earth's Greenhouse**
 - **Venus** has an actual average temperature of 450 °C vs. 100 °C if no greenhouse effect
 - **Earth** has an actual average temperature of 15 °C vs. -18 °C if no green house effect

- **Greenhouse Gasses**
 - **CO₂, H₂O, CFCs**, etc.

3B Changes in CO₂ Over Time

- Graphics from Text: Figure 3.1, Atmospheric CO₂ changes over the last 160,000 years
 - Note: the correlation between temperatures and [CO₂]
 - Note: the waxing and waning of the Ice Ages
 - How measured?

- Graphics from Text: Figure 3.3, Mona Loa [CO₂]
 - Note: The seasonal variations and longer term trends in [CO₂]

- Graphics from Text: Figure 3.4 in 2nd Edition and 3.5 in 3rd Edition, Average measured temperature changes at the earth's surface
 - How measured?

- Graphics from Text: Figure 3.4 in the 3rd Edition, predicted trends in CO₂ emissions

➤ How estimated?

➤ Dynamic Balance of CO₂

➤ Photosynthesis



➤ Respiration



➤ Longer term processes

➤ Biomass

➤ Fossil Fuels

➤ Carbonate Minerals (e.g., Calcium Carbonate)



➤ Graphics from Text: Figure 3.8 in 2nd Edition and 3.9 in 3rd

Edition, the Carbon Cycle

3C Molecules: How They Shape Up

➤ How do we know **molecular shapes**?

Experimental Observations of Shapes



Measurements of Bond Lengths and Bond Angles



Correlations with Bonding Theories



Predictions of Shapes for New Molecules

- Observed **Molecular Shapes**
 - General Features of Structures

 - **Complex 3D Shapes**
 - **109.5°, 120°, and 180° Bond Angles**
 - correlated with the number of groups around an atom

 - **1.2 – 1.55 Å Bond Distances (C-H ≈ 1 Å)**
 - Correlated with **Bond Order**

- **Structural Correlations with Properties**

➤ VSEPR, Valence Shell Electron Pair Repulsion Theory

➤ Molecular shapes \Rightarrow Bond Angles

➤ Each “thing” is an attached atom or a lone pair

➤ Four things \Rightarrow Tetrahedral, td, 109.5°

➤ Three things \Rightarrow Trigonal planar, 120°

➤ Two things \Rightarrow Linear, 180°

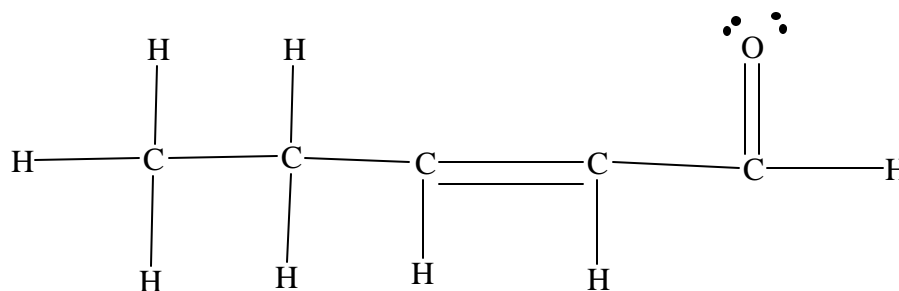
➤ Bond Distances

➤ Single Bonds \Rightarrow Long Distances

➤ Double Bonds \Rightarrow Medium Distances

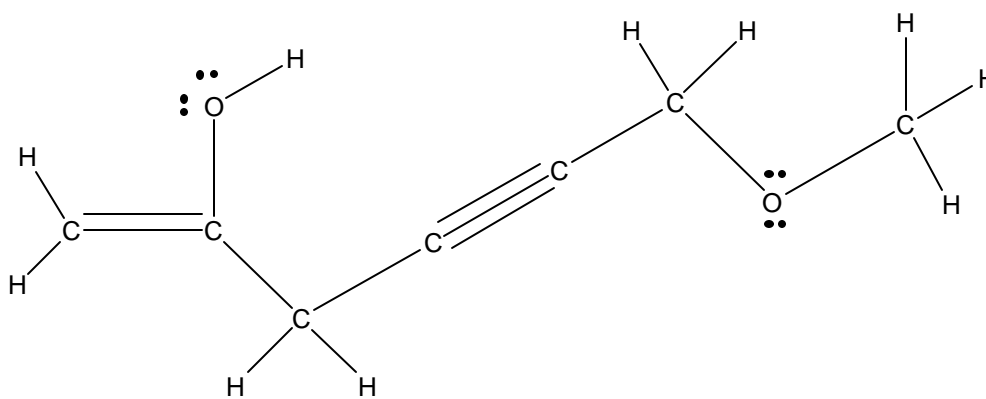
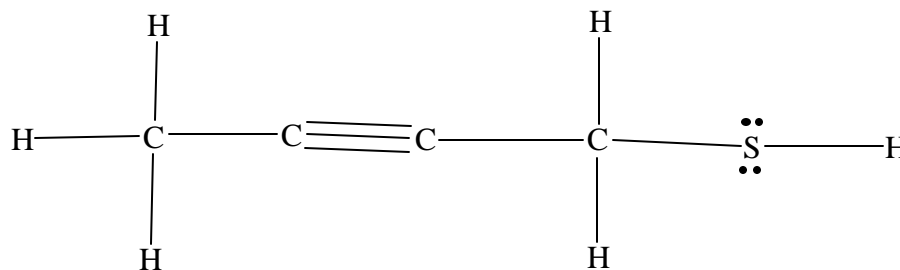
➤ Triple Bonds \Rightarrow Short Distances

➤ Example



➤ Ask Students: Predict the bond lengths and angles in the following molecules

➤ Group Activity



3D Vibrating Molecules

- The atoms in molecules never sit still with respect to one another
- They constantly **vibrate** as if held together by springs
- Once they start vibrating, the rate of vibration (i.e., its **frequency**) doesn't change
- Each molecules can only vibrate at certain **specific frequencies**

- When a molecule is hit by a **photon of light** having the same energy as the energy difference between two vibration, the vibration rate will “**jump up**”
- If a vibration rate slows down to a new rate, then a photon having the **energy difference** will be given off

- **Vibration Frequencies and Molecular Structures**
- Stronger bonds vibrate at higher frequencies
 - Weaker bonds vibrate at lower frequencies
- Heavier atoms vibrate at lower frequencies
 - Lighter atoms vibrate at higher frequencies
- Molecular structure effects the number and energy of vibrations
- The balance of these trends produces **molecular spectra**
 - No two of these are identical

- The more complex the molecular structure, the greater the number of vibrations that will occur
- In the **Infra-Red (IR)** region of the **electromagnetic spectrum**

- **Graphics from Text: Figure 3.5 in 2nd Edition and 3.6 in 3rd Edition, IR Spectrum of CO₂**
 - **CO₂** has a simple structure and therefore a simple spectrum

- **Graphics from Text: Figure 3.6 in 2nd Edition and 3.7 in 3rd Edition, IR Spectrum of H₂O**
 - **H₂O** has a more complex structure and therefore a more complex spectrum

- **Graphics from Text: Figure 3.7 in 2nd Edition and 3.8 in 3rd Edition, Molecular responses to various types of electromagnetic energy**

3E Weighing Substances

- One can determine the weight of individual molecules or collections of molecules
- Steps to calculate the **Molecular Weight, MW**, of the substance
 - 1st, find the **atomic weight** of each atom in the substance
 - 2nd, multiply the weight of each atom by the number of atoms of that type to give the total weight of each **element**
 - 3rd, add the total weights of all of the elements
 - 4th, this number is in **AMU (Atomic Mass Units)** for **individual atoms** and **grams for moles of atoms**
- Examples:
 - Calculate the MW of $\text{CO}_2 \Rightarrow 12 + 2(16) = 44$
 - Calculate the MW of $\text{CH}_2\text{F}_2 \Rightarrow 12 + 2(1) + 2(19) = 52$

- One can determine the **Percent Composition** of individual molecules and collections of molecules
- Steps to calculate Percent Composition
 - 1st, get the **MW**
 - 2nd, get the total **weight of the element** in that molecule
 - 3rd, divide the total weight of that element by the MW and multiply by 100 to get percentage
 - 4th, repeat for all elements
- Example:
 - Calculate the %C, %H, and %F of **CH₂F₂** (remember **MW** = 52)
 - %C $\Rightarrow 12 / 52 \times 100 = 23.1\%$
 - %H $\Rightarrow 2 / 52 \times 100 = 3.8\%$
 - %F $\Rightarrow 38 / 52 \times 100 = 73.1\%$

➤ Ask Students: Calculate the MW and Elemental

Compositions of the following molecules

➤ Group Activity

➤ CS_2

➤ MW =

➤ %C =

➤ %S =

➤ $\text{C}_3\text{H}_2\text{F}_4$

➤ MW =

➤ %C =

➤ %H =

➤ %F =

3F Calculating with Moles

- Determining the number of **moles** of a substance you have
 - Steps:
 - Determine the **Molecular Weight** of the substance
 - Determine the **Weight** of the substance
 - Divide the two numbers, i.e., # **Moles** = $\text{Weight} / \text{MW}$

- Determining the number of **grams** of a substance you have
 - Steps:
 - Determine the **Molecular Weight** of the substance
 - Determine the number of moles of the substance
 - Divide the two numbers, i.e., $\text{Weight} = \# \text{Moles} \times \text{MW}$

- Examples (For each of the following, determine the number of moles or weight of the substance, as required):
 - For **CH₂F₂** (MW = 52)

➤ Ask Students: For each of the following, determine the number of moles or weight of the substance, as required

➤ Group Activity

➤ CS_2 20 g

➤ CS_2 0.24 moles

➤ $\text{C}_3\text{H}_2\text{F}_4$ 11.5 g

➤ $\text{C}_3\text{H}_2\text{F}_4$ 11.6 moles

3G Humans and CO₂

➤ Ask Students: Estimate the number of tons of CO₂ produced by your car each year

➤ Group and Board Activity

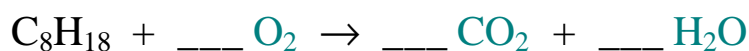
➤ Steps:

➤ Number of gallons of gas you add each week = ?

➤ Assume each gallon of gas weighs about 4 kg

➤ Assume that the formula for gasoline is C₈H₁₈ (i.e., pure Octane)

➤ Balance the reaction for combustion



➤ From the number of kg of Octane, calculate the number of moles of octane

➤ From the number of moles of Octane, calculate the number of moles of CO₂

➤ From the number of moles of CO₂, calculate its weight

- Given the number of cars in the world, one can easily see that we release a lot of CO₂

- Human effects on CO₂ balance
 - People release a total of about 6 - 7 billion tons per year
 - 5 billion tons from fossil fuels
 - 1 - 2 billion tons from deforestation

- CO₂ levels
 - 290 ppm before the Industrial Revolution
 - 360 ppm in 2000
 - net increase of 1.5 ppm per year

- of total CO₂ people release
 - one half is lost to Biosphere and Geosphere
 - this leaves about 3 billion tons added per year (i.e., 1.5 ppm or 740 billion metric tons)

3H Methane and Global Warming

- Remember: **Methane** has more peaks in its IR than does **CO₂**
 - It therefore is a stronger **greenhouse gas** (about 15 - 30 times)

- Sources of **Methane**
 - **Swamps** (marsh gas)
 - **Rice Paddies**
 - **Ruminant** (cattle, sheep) **flatulence** (73 million tons per year)
 - **Termites** (about 0.5 tonnes of termites per person)
 - **Natural Gas** production leaks

- **Clathrates**
 - **Methane ices**
 - **Arctic permafrost**
 - **Sea Beds**
 - **Fuels?**
 - **Non-linear effects**

3I Where do we go from here: Climate Modeling and Future

Changes

- Climatic Modeling
 - Limits to its accuracy
 - Program limitations
 - Computer limitations
 - Science understanding limitations
 - Data limitations
 - What it does
 - General predictions
 - Average temperature changes
 - Changes in extreme temperatures
 - Rainfall changes
 - Sources of political controversy, differential costs/benefits

Index of Vocabulary and Major Topics

<i>I</i>		Correlations with Bonding.....	6
[CO ₂]	4	costs/benefits.....	21
<i>I</i>		CS ₂	15, 17
109.5°	7, 8	<i>D</i>	
120°	7	Distances.....	8
180°	7	Double Bonds.....	8
<i>A</i>		Dynamic Balance of CO ₂	5
AMU.....	13	<i>E</i>	
Arctic permafrost.....	20	Earth.....	3
Ask Students.....	9, 15, 17, 18	Earth's Greenhouse.....	3
atmosphere.....	3	electromagnetic energy.....	12
Atmospheric CO ₂ changes over the last 160,000 years.....	4	electromagnetic spectrum.....	12
Atomic Mass Units.....	13	element.....	13
atomic weight.....	13	Elemental Compositions.....	15
<i>B</i>		energy difference.....	10
Biomass.....	5	Experimental Observations.....	6
Biosphere.....	19	<i>F</i>	
Bond Angles.....	6, 7, 8	flatulence.....	20
Bond Distances.....	7, 8	Fossil Fuels.....	5
Bond Lengths.....	6	frequencies.....	11
Bond Order.....	7	frequency.....	10
<i>C</i>		Fuels.....	20
C ₃ H ₂ F ₄	15, 17	<i>G</i>	
C ₆ H ₁₂ O ₆	5	gardening.....	3
C ₈ H ₁₈	18	Geosphere.....	19
Ca(CO ₃).....	5	Glucose.....	5
Ca ⁺²	5	gram.....	13, 16
Calcium Carbonate.....	5	Graphics from Text.....	3, 4, 5, 12
Calculate the MW.....	13	greenhouse.....	3
Calculating with Moles.....	16	greenhouse gas.....	20
Carbon Cycle.....	5	Greenhouse Gasses.....	3
Carbonate Minerals.....	5	Group Activity.....	9, 15, 17
cattle.....	20	Group and Board Activity.....	18
CFC.....	3	<i>H</i>	
CH ₂ F ₂	13, 14, 16	H ₂ O.....	3, 5, 12, 18
Changes in CO ₂ Over Time.....	4	Humans and CO ₂	18
Clathrates.....	20	<i>I</i>	
Climatic Modeling.....	21	Ice Ages.....	4
CO ₂	3, 5, 12, 13, 18, 20	individual atoms.....	13
CO ₂ balance.....	19	Industrial Revolution.....	19
CO ₂ levels.....	19	Infra-Red.....	12
combustion.....	18	IR.....	12
Complex 3D Shapes.....	7	IR Spectrum of CO ₂	12

IR Spectrum of H₂O..... 12

J

jump up 10

L

Light Energy 5

Limits to its accuracy 21

M

marsh gas..... 20

measured temperature changes 4

Methane 20

Methane and Global Warming..... 20

Methane ices 20

mole..... 16

molecular shapes 6

Molecular Shapes 7

molecular spectra..... 11

Molecular Structures..... 11

Molecular Weight..... 13, 16

Molecules: How They Shape Up..... 6

Moles 16

moles of atoms..... 13

Mona Loa..... 4

MW..... 13, 14, 16

N

Natural Gas..... 20

Non-linear effects..... 20

O

O₂ 5, 18

Octane 18

P

Percent Composition..... 14

photon of light..... 10

Photosynthesis 5

political controversy 21

Predict the bond lengths and angles 9

predicted trends in CO₂ emissions..... 4

Predictions of Shapes 6

R

Rainfall changes 21

Respiration 5

Rice Paddies 20

Ruminant 20

S

Sea Beds..... 20

sea water 5

sheep..... 20

Single Bonds..... 8

specific frequencies 10

spectrum..... 12

Structural Correlations with Properties 7

Swamps..... 20

T

td 8

temperature changes 21

Termites 20

Tetrahedral..... 8

The Greenhouse Effect..... 3

thing..... 8

total CO₂ people release..... 19

Trigonal planar 8

Triple Bonds..... 8

V

Valence Shell Electron Pair Repulsion Theory 8

Venus..... 3

vibrate..... 10

Vibrating Molecules 10

Vibration Frequencies 11

VSEPR..... 8

W

Weighing Substances 13

weight of the element 14

Where do we go from here: Climate Modeling and
Future Changes..... 21