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

- 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
  - CO_2, H_2O, CFCs, etc.

3B Changes in CO_2 Over Time

- Graphics from Text: Figure 3.1, Atmospheric CO_2 changes over the last 160,000 years
  - Note: the correlation between temperatures and [CO_2]
  - Note: the waxing and waning of the Ice Ages
  - How measured?

- Graphics from Text: Figure 3.3, Mona Loa [CO_2]
  - Note: The seasonal variations and longer term trends in [CO_2]

- 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 CO_2 emissions

- How estimated?

- Dynamic Balance of CO_2
  - Photosynthesis

$$6\,CO_2 + 6\,H_2O + \text{Light Energy} \rightarrow C_6H_{12}O_6\ (\text{Glucose}) + 6\,O_2$$

  - Respiration

$$C_6H_{12}O_6 + 6\,O_2 \rightarrow 6\,CO_2 + 6\,H_2O + \text{Energy}$$

  - Longer term processes
    - Biomass
    - Fossil Fuels
    - Carbonate Minerals (e.g., Calcium Carbonate)

$$CO_2 + Ca^{+2}\ (\text{sea water}) \rightarrow Ca(CO_3) \downarrow$$

  - 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

⇓

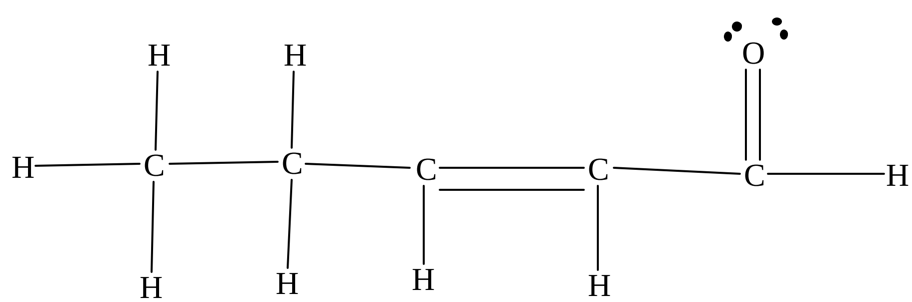
Predictions of Shapes for New Molecules

- 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

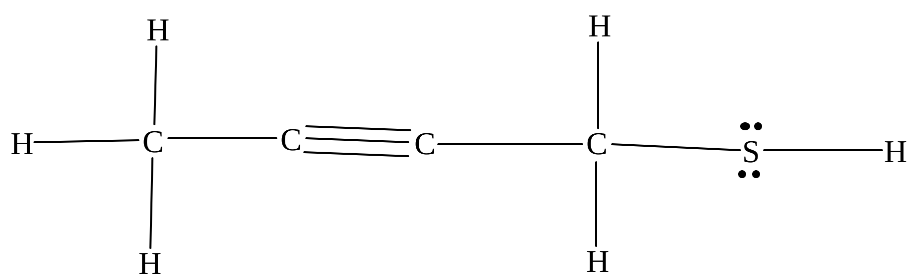
- VSEPR, Valence Shell Electron Pair Repulsion Theory
  - Molecular shapes ⇒ Bond Angles
    - Each "thing" is an attached atom or a lone pair
    - Four things ⇒ Tetrahedral, td, 109.5°
    - Three things ⇒ Trigonal planar, 120°
    - Two things ⇒ Linear, 180°

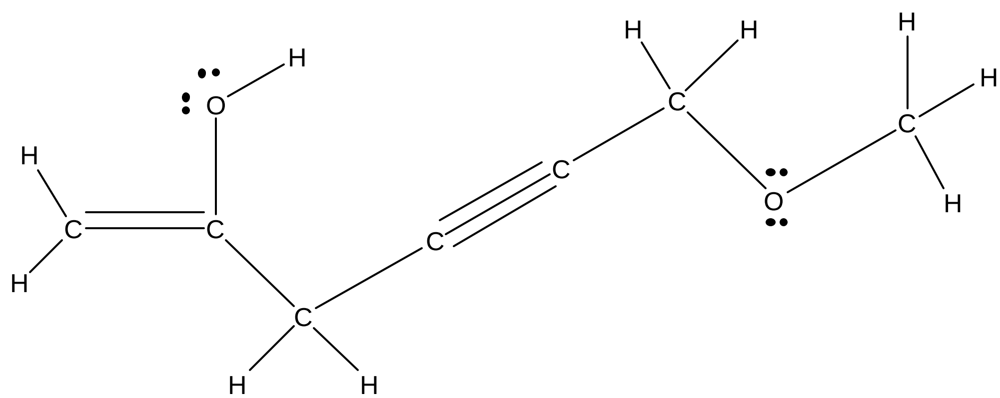
- Bond Distances
    - Single Bonds ⇒ Long Distances
    - Double Bonds ⇒ Medium Distances
    - Triple Bonds ⇒ Short Distances

- 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 a lower frequencies
    - Lighter atoms vibrate a 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 CO_2
  - CO_2 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 H_2O
  - H_2O 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 $CO_2 \Rightarrow 12 + 2(16) = 44$
    - Calculate the MW of $CH_2F_2 \Rightarrow 12 + 2(1) + 2(19) = 52$

- 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 CH_2F_2 (remember MW = 52)
    - %C $\Rightarrow$ 12 / 52 x 100 = 23.1%
    - %H $\Rightarrow$ 2 / 52 x 100 = 3.8%
    - %F $\Rightarrow$ 38 / 52 x 100 = 73.1%

- Ask Students: Calculate the MW and Elemental Compositions of the following molecules
  - Group Activity
  - CS_2
    - MW =
    - %C =
    - %S =
  - $C_3H_2F_4$
    - 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 = Weight / 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., Weight = # Moles x MW

- Examples (For each of the following, determine the number of moles or weight of the substance, as required):
  - For CH_2F_2 (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
  - $C_3H_2F_4$ 11.5 g
  - $C_3H_2F_4$ 11.6 moles

3G Humans and CO_2

- Ask Students: Estimate the number of tons of CO_2 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 C_8H_{18} (i.e., pure Octane)
      - Balance the reaction for combustion

$$C_8H_{18} + \_\_\_ \ O_2 \rightarrow \_\_\_ \ CO_2 + \_\_\_ \ H_2O$$

      - 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 CO_2
      - From the number of moles of CO_2, calculate its weight

- Given the number of cars in the world, one can easily see that we release a lot of CO_2

- Human effects on CO_2 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

  - CO_2 levels
    - 290 ppm before the Industrial Revolution
    - 360 ppm in 2000
    - net increase of 1.5 ppm per year

  - of total CO_2 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 CO_2
    - 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

- Clatherates
    - 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

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