Example: Line structure/formula

- Find molecular formula
- Find molar mass

N-acetyl-para-aminophenol (tylenol)
Formulas & % composition

- Given a chemical formula, it is easy to calculate the mass % for each element.
- Just find molar mass of molecule and the amount contributed by each element.
- As an example, we’ll calculate mass % of each element in the “tylenol molecule”.

Composition & formulas

- The reverse process is useful in analyzing unknown substances.
- Instruments are available which can tell us the elemental composition of a substance. (“elemental analysis”)
- We can convert this info into a molecular formula.
Composition & formulas: example

- Nicotine contains 74.0% C, 8.65% H, and 17.35% N. If the molar mass of nicotine is 162, what is the chemical formula of nicotine?

- Atomic weights are 12, 1, and 14 for C, H, and N. (More precisely, they are 12.01, 1.008, and 14.01 g/mol, respectively.)

Nicotine structure

Nicotine
\( C_{10}H_{14}N_2 \)
Empirical vs. Molecular formula

- Last example shows difference between empirical and molecular formulas.
- **Empirical formula:** simplest possible formula with correct ratios of atoms
- **Molecular formula:** formula showing the actual composition of a molecule
- Can find molecular formula from empirical formula if we know molar mass

Formulas from % composition; more examples

- Hydrogen peroxide is 5.93% hydrogen and 94.07% oxygen by weight. What is its chemical formula?
- An unknown sample of a pure substance is 43.7% P and 56.3% O by weight. What is its chemical formula?

Note: mass ratios do not give mole ratios, since atomic masses are not the same.
Quantity of $\text{CO}_2$ yields the carbon composition; quantity of $\text{H}_2\text{O}$ yields the hydrogen composition. If only C, H & O - get O by difference.

eg.: Ethylbutanoate contains only C, H, and O. Combustion of a 50 g sample gave 114 g $\text{CO}_2$ and 46.6 g $\text{H}_2\text{O}$. If the molar mass of ethylbutanoate is ~116g, what is its molecular formula?
**Chemical Reactions**

- Transformation of one or more chemical species into new substances.
- “reactants” → “products”
- Planning a synthesis is a “chemical design” problem.

**Chemical Equations**

- Written description of a reaction
- Varying levels of information: physical states, conditions, etc.
- Doesn’t necessarily mean that the reaction will take place readily, or at all.

\[
C \text{(diamond)} + O_2(g) \rightarrow CO_2(g)
\]
A Few Types of Reactions
(unbalanced equations!)

- “addition” or “combination” reactions
  \[ \text{C}_2\text{H}_4 + \text{H}_2 \rightarrow \text{C}_2\text{H}_6 \]
- “decomposition” reactions
  \[ \text{NH}_4\text{NO}_3 \rightarrow \text{N}_2 + \text{O}_2 + \text{H}_2\text{O} \]
- “substitution” or “displacement” reactions
  \[ \text{Mg} + \text{HCl} \rightarrow \text{MgCl}_2 + \text{H}_2 \]

More Types of Reactions
(unbalanced equations!)

- “combustion” reactions (burning in \( \text{O}_2 \))
  \[ \text{C}_4\text{H}_{10} + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O} \]
- acid-base reactions  (next week)
- precipitation reactions  (next week)
- oxidation-reduction reactions
Balancing Equations: Conservation Laws

• In any chemical reaction, the following are conserved, and can be “accounted for.”
  ➔ number of atoms of each element
  ➔ mass
  ➔ energy
  ➔ electric charge

Meaning of “Balanced” Equations

\[ 2 \text{ CO} + \text{O}_2 \rightarrow 2 \text{ CO}_2 \]

• Coefficients give “reaction ratio”, and tell us how many ...
  ➔ Molecules react with molecules
  ➔ Moles react with moles
  ➔ **NOT how many grams react with grams!!!**
Balancing Equations

- Find smallest whole number coefficients that satisfy conservation rules
- For many reactions, we do this “by inspection.” (trial and error)
- For some reactions, often use more systematic methods (redox reactions).

For example...

- Burning of propane \((C_3H_8)\) from a propane tank:
  \[ C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O \]
“Stoichiometry”

- Quantitative relationships in chemistry: “How much” or “How many” questions
- Applications of conservation laws
- “Composition stoichiometry” vs. “Reaction Stoichiometry”

Reaction Stoichiometry

- Balanced equation!
- “Moles react with moles.”
  - calculations centered on moles
- Use sample weight, molecular weight (molar mass), volume, density, etc. to relate known info to # of moles.
Example:

\[ 2 \text{C}_2\text{H}_2 + 5 \text{O}_2 \rightarrow 4 \text{CO}_2 + 2 \text{H}_2\text{O} \]

How many grams of \( \text{O}_2 \) are required to burn 52 g of \( \text{C}_2\text{H}_2 \)?