Chapter 9

Chemical Calculations and Chemical Formulas

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Making Phosphoric Acid

- Furnace Process for making H₃PO₄ to be used to make fertilizers, detergents, and pharmaceuticals.
 - React phosphate rock with sand and coke at 2000 °C. $2Ca_3(PO_4)_2 + 6SiO_2 + 10C$ $\rightarrow 4P + 10CO + 6CaSiO_3$
 - React phosphorus with oxygen to get tetraphosphorus decoxide.

 $4P + 5O_2 \rightarrow P_4O_{10}$

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React tetraphosphorus decoxide with water to make phosphoric acid.

 $P_4O_{10} + 6H_2O \rightarrow 4H_3PO_4$

Sample Calculations (1)

- What is the maximum mass of P_4O_{10} that can be formed from 1.09×10^4 kg P?
- The formula for P_4O_{10} provides us with a conversion factor that converts from units of P to units of P_4O_{10} .

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 $(1 \text{ molecule } P_4O_{10})$

4 atoms P

Sample Calculations (2)

• What is the minimum mass of water that must be added to 2.50×10^4 kg P₄O₁₀ to form phosphoric acid in the following reaction?

 $P_4O_{10} + 6H_2O \rightarrow 4H_3PO_4$

• The coefficients in the balanced equation provide us with a conversion factor that converts from units of P_4O_{10} to units of H_2O .

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6 molecules H_2O

 $1 \text{ molecule } P_4O_{10}$

Goal: To develop conversion factors that will convert between a measurable property (mass) and number of particles

Measurable Property 1 Number of Particles 1 Number of Particles 2 Measurable Property 2

Mass 1 \downarrow Number of Particles 1 \downarrow Number of Particles 2 \downarrow Mass 2

Counting by Weighing for Nails

- Step 1: Choose an easily measurable property.
 - Mass for nails
- Step 2: Choose a convenient unit for measurement.
 - Pounds for nails

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Counting by Weighing for Nails (cont)

- Step 3: If the measurable property is mass, determine the mass of the individual objects being measured.
 - Weigh 100 nails: 82 are 3.80 g, 14 are 3.70 g, and 4 are 3.60 g
- Step 4: If the objects do not all have the same mass, determine the weighted average mass of the objects.
 0.82(3.80 g) + 0.14(3.70 g) + 0.04(3.60 g) = 3.78 g

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Counting by Weighing for Nails (cont)

• Step 5: Use the conversion factor from the weighted average to make conversions between mass and number of objects.

? nails = 218 lb nails
$$\left(\frac{453.6 \text{ g}}{1 \text{ lb}}\right) \left(\frac{1 \text{ nail}}{3.78 \text{ g nails}}\right) = 2.62 \times 10^4 \text{ nails}$$

Counting by Weighing for Nails (cont)

 Step 6: Describe the number of objects in terms of a collective unit such as a dozen, a gross, or a ream.

$$\frac{? \text{ g nails}}{1 \text{ gross nails}} = \left(\frac{3.78 \text{ g nails}}{1 \text{ nail}}\right) \left(\frac{144 \text{ nails}}{1 \text{ gross nails}}\right) = \frac{544 \text{ g nails}}{1 \text{ gross nails}}$$

$$? \text{ gross nails} = 218 \text{ lb nails} \left(\frac{453.6 \text{ g}}{1 \text{ lb}}\right) \left(\frac{1 \text{ gross nails}}{544 \text{ g nails}}\right) = 182 \text{ gross nails}$$

Counting by Weighing for Carbon Atoms

- **Step 1:** Choose an easily measurable property.
 - Mass for carbon atoms

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- Step 2: Choose a convenient unit for measurement.
 - Atomic mass units (u) for carbon atoms
 - Atomic mass unit (u) = 1/12 the mass of a carbon-12 atom (with 6 p, 6 n, and 6 e⁻)

Counting by Weighing for Carbon Atoms (cont)

• Step 3: If the measurable property is mass, determine the mass of the individual objects being measured.

- For carbon: 98.90% are 12 u and 1.10% are 13.003355
- Step 4: If the objects do not all have the same mass, determine the weighted average mass of the objects.
 0.9890(12 u) + 0.0110(13.003355 u) = 12.011 u

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Counting by Weighing for Carbon Atoms (cont)

 Step 5: Describe the number of objects in terms of a collective unit such as a dozen, a gross, or a ream, and use this and the weighted average to create a conversion factor to make conversions between mass and number of objects.

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Mole

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- A *mole* (mol) is an amount of substance that contains the same number of particles as there are atoms in 12 g of carbon-12.
- To four significant figures, there are 6.022×10^{23} atoms in 12 g of carbon-12.
- Thus a mole of natural carbon is the amount of carbon that contains 6.022×10^{23} carbon atoms.
- The number 6.022 × 10²³ is often called *Avogadro's number*.

Avogadro's Number



Molar Mass Development

From the definition of an unified atomic mass unit, u $\frac{12 \text{ u C-12}}{1 \text{ atom C-12}}$ From the definition of mole $\frac{12 \text{ g C-12}}{1 \text{ mol C-12}}$ From relative atomic masses $\frac{12.011 \text{ g C}}{1 \text{ mol C}}$ $\frac{24.3050 \text{ g Mg}}{1 \text{ mol Mg}}$ $\frac{15.9994 \text{ g O}}{1 \text{ mol O}}$ $\frac{1.00794 \text{ g H}}{1 \text{ mol H}}$

Molar Mass For Elements

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Atomic Mass from the Periodic Table

(atomic mass) g element 1 mol element

Molar Mass Calculation for Carbon

? mol C = 0.55 carat
$$\left(\frac{1 \text{ g}}{5 \text{ carat}}\right) \left(\frac{1 \text{ mol C}}{12.011 \text{ gC}}\right) = 9.2 \times 10^{-3} \text{ mol C}$$

Goal: To develop conversion factors that will convert between a measurable property (mass) and number of particles

Measurable Property 1 Number of Particles 1 Number of Particles 2 Measurable Property 2 Mass 1 \downarrow Moles 1 \downarrow Moles 2 \downarrow Mass 2

Molecular Mass

• Whole = sum of parts

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- mass of a molecule = sum of the masses of the atoms in the molecule
- molecular mass = the sum of the atomic masses of the atoms in the molecule

Molar mass O: 15.9994 g/mol Molar mass H: 1.00794 g/mol 1.00794 g/mol

Molar mass H₂O: 18.0153 g/mol

Molar Mass For Molecular Compounds

 Molecular Mass = Sum of the atomic masses of atoms in one molecule

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(molecular mass) g molecular compound 1 mol molecular compound

Formula Units

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- A formula unit of a substance is the group represented by the substance's chemical formula, that is, a group containing the kinds and numbers of atoms or ions listed in the chemical formula.
- Formula unit is a general term that can be used in reference to elements, molecular compounds, or ionic compounds.

Formula Unit Examples



contains one Ne atom.

liquid water (molecular compound)



Liquid water is composed of discrete H₂O molecules.

A formula unit of water contains one oxygen atom and two hydrogen atoms. ammonium chloride (ionic compound)



There are no separate ammonium chloride, NH_4Cl , molecules. Each ion is equally attracted to eight others. A formula unit of ammonium chloride contains one ammonium ion, NH_4^+ , and one chloride ion, Cl^- , (or one nitrogen atom, four hydrogen atoms, and one chloride ion).

Formula Mass for Ionic Compounds

- Whole = sum of parts
- Mass of a formula unit = sum of the masses of the atoms in the formula unit
- Formula mass = the sum of the atomic masses of the atoms in the formula



Molar Mass For Ionic Compounds

 Formula Mass = Sum of the atomic masses of the atoms in a formula unit

(formula mass) gionic compound 1 mol ionic compound

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Molar Mass Development

From the definition of an unified atomic mass unit, u		12 u C-12
		1 atom C-12
From the definition of mole $\frac{1}{1}$	12 g C-12 mol C-12	
From relative atomic masses		
12.011 g C 24.3050 g Mg 1 mol C 1 mol Mg	15.9994 g O 1 mol O	1.00794 g H 1 mol H
From relative molecular masses	18.0153 g H ₂ O 1 mol H ₂ O	
From relative formula masses	58.4425 g NaCl 1 mol NaCl	

General Conversions



Units of One Substance to Units of Another



Study Sheets

- Write a description of the "tip-off" that helps you to recognize the type of problem the calculation represents.
- Write a description of the general procedure involved in the particular type of problem.
- Write an example of the type of calculation.

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Sample Study Sheet: Converting Between Mass of Element and Mass of Compound Containing the Element

• **Tip-off:** When you analyze the type of unit you have and the type of unit you want, you recognize that you are converting between a unit associated with an element and a unit associated with a compound containing that element.

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Sample Study Sheet (2)

General Steps

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- Convert the given unit to moles of the first substance.
- Convert moles of the first substance to moles of the second substance using the molar ratio derived from the formula for the compound.
- Convert moles of the second substance to the desired units of the second substance.



Calculating Empirical Formulas

Step 1: If you are not given mass in grams for each element, convert the data you are given to grams of each element.

- This may involve simple unit conversions. For example, you may be given pounds or milligrams, which you convert to grams using dimensional analysis.
- Sometimes you are given the percentage of each element in the compound. Assume that you have 100 g of compound, and change the units of the values given for the percentages to grams.

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Calculating Empirical Formulas

Step 2: Convert grams of each element to moles by dividing by the atomic mass of the element.
Step 3: Divide each mole value by the smallest and round your answers to whole numbers or common mixed fractions.

Step 4: If you have a fraction after the last step, multiply all the mole values by the denominator of the fraction.

Step 5: The resulting mole values correspond to the subscripts in the empirical formula.

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Simplest molar ratio (empirical formula)

Calculating Molecular Formulas

Step 1: If necessary, calculate the empirical formula of the compound from the data given.

Step 2: Divide the given molecular mass by the empirical formula mass.

 $n = \frac{molecular mass}{empirical formula mass}$

Step 3: Multiply each of the subscripts in the empirical formula by n to get the molecular formula.

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Calculating Molecular Formulas Image

