Calculations involving concentrations, stoichiometry

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Metric System Units

- Meter (m), gram (g), liter (l), second (s)
- Prefixes:
  - mega- M 1,000,000 (10^6)
  - kilo- k 1000 (10^3)
  - deci- d 0.1 (10^{-1})
  - centi- c 0.01 (10^{-2})
  - milli- m 0.001 (10^{-3})
  - micro- µ 0.000001 (10^{-6})
  - nano- n 0.000000001 (10^{-9})
  - pico- p 0.000000000001 (10^{-12})
**Significant figures in calculations:**

- **Multiplication or division:**
  Keep smallest number of significant figures in answer

- **Addition or subtraction:**
  Keep smallest number of decimal places in answer

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**Mole**

- Unit of amount of substance
- **the amount of substance containing as many particles (atoms, ions, molecules, etc.) as present in 12 g of the carbon isotope \( ^{12}\text{C} \)**
- this amount equals 6.02 x \(10^{23}\) particles (Avogadro’s Number)
(Relative) Atomic Weight

- atomic mass unit (u): 1/12 of the mass of one atom of the carbon isotope $^{12}\text{C}$
  
  \[ 1 \text{ u} = 1.66057 \times 10^{-27} \text{ kg} \]

- relative atomic mass (atomic weight, AW): mass of an atom expressed in u

- molecules: (relative) molecular mass (molecular weight, MW)

- substances that do not form true molecules (ionic salts etc.): (relative) formula weight (FW)

Ionic salts: no true molecule

- Crystal lattice of NaCl:

- Dissolution of NaCl in water: electrolytic dissociation producing hydrated independent ions Na$^+$, Cl$^-$

Formula unit
Molar Mass

- mass of one mole of given substance
- expressed in g/mol
- The molar mass of a substance in grams has the same numerical value as its relative atomic (molecular) weight

Molar Volume

One mole of any gaseous substance occupies the same volume at the same temperature and pressure.

\[ 22.414 \text{ litres} \text{ at } 101.325 \text{ kPa, } 0 \, ^{\circ}\text{C} (273.15 \text{ K}) \]
(Avogadro’s Law)
\[
P \cdot V = n \cdot R \cdot T
\]

P: pressure in kPa
V: volume in dm\(^3\) (l)
n: number of moles
R: universal gas constant (8.31441 N.m.mol\(^{-1}\).K\(^{-1}\))
T: temperature in K

Example: what is volume of one mole of gas at 101.325 kPa and 25 °C ?

\[
V = \frac{n \cdot R \cdot T}{P} = \frac{1 \times 8.31441 \times (273.15+25)}{101.325} = 24.465 \text{ dm}^3
\]
Solution

• homogeneous dispersion system of two or more chemical entities whose relative amounts can be varied within certain limits
• solvent + solute(s)
• gaseous (e.g. air)
• liquid (e.g. saline, NaCl dissolved in water)
• solid (e.g. metal alloy)

Concentration of a solution

• Mass concentration: grams of dissolved substance per liter of solution

• Molar concentration: moles of dissolved substance per liter of solution
Conversion from mass to molar

Example: Calculate molar concentration of Na$_2$HPO$_4$ solution $c = 21$ g/l.
(AW of Na: 23, P: 31, O: 16, H: 1)

FW of Na$_2$HPO$_4$: 46 + 1 + 31 + 4x16 = 142
Molar concentration = Mass conc. (g/l) / FW
= 21 / 142 = 0.15 mol/l

Conversion from molar to mass

Example: Calculate how many g of KClO$_4$ is needed for preparation of 250 ml of 0.1 M solution.
(AW of K: 39, Cl: 35.4, O: 16)

FW of KClO$_4$: 39 + 35.4 + 4x16 = 138.4
Mass conc. = molar conc. x FW
we need 138.4 x 0.1 x 0.25 = 3.46 g KClO$_4$
Conversions between mass and molarity: Summary

- Always distinguish between amount of substance in moles (grams) and concentration of substance in mol/l (g/l)
- For conversion from mass to molarity divide the mass (g or g/l) with molar mass (relative AW/MW/FW)
- For conversion from molarity to mass multiply the molarity (mol or mol/l) with molar mass (relative AW/MW/FW)

Concentration of a solution in %

% weight per weight (w/w): grams of substance in 100 g of mixture

\[= \frac{\text{mass of solute}}{\text{mass of solution}} \times 100\]

% weight per volume (w/v): grams of substance in 100 ml of solution

\[= \frac{\text{mass of solute in g}}{\text{volume of sol. in ml}} \times 100\]

% volume per volume (v/v): ml of substance in 100 ml of solution

\[= \frac{\text{volume of solute}}{\text{volume of solution}} \times 100\]
Conversion from % to molarity

Example: The physiological saline is NaCl 0.9 % (w/v)
What is molar concentration of NaCl in this solution?
(AW of Na: 23, Cl: 35.5)

FW of NaCl : 23+35.45 = 58.5
0.9 % (w/v) is 0.9 g/100 ml = Mass conc. 9 g/l
Molar concentration = Mass conc. (g/l) / FW
= 9/58.5 = 0.15 mol/l

Diluting solutions

Example: How many ml of water should be added to 100 ml of NaCl 1 mol/l, in order to get 0.15 mol/l (‘physiological saline’)?

\[ c_1 \cdot v_1 = c_2 \cdot v_2 \]
\[ 1 \times 100 = 0.15 \times v_2 \]
\[ v_2 = 100/0.15 = 666.67 \text{ ml} \]

Volume that needs to be added:
666.67 ml - 100 ml = \textbf{566.67 ml}
Diluting solutions

Example II: You need to prepare 1 liter of 0.1 M HCl. How many ml of concentrated HCl (12 M) do you need to take?

\[ c_1 \cdot v_1 = c_2 \cdot v_2 \]

\[ 12 \times v_1 = 0.1 \times 1000 \]

\[ v_1 = \frac{100}{12} = 8.33 \text{ ml} \]

What is molarity of pure water?

Molar concentration: moles of substance per liter of solution

1 liter of water weighs 997 g at 25 °C

FW of \( \text{H}_2\text{O} \): 2+16=18

997 g \( \text{H}_2\text{O} \) is \( \frac{997}{18} = 55.4 \) moles

Molarity of pure water is **55.4 mol/l**
Calculations with molar volume

Example: What is weight (in grams) of 1 liter of oxygen at atmospheric pressure and ambient temperature?
(AW of O: 16)

Molar volume at 101.325 kPa and 25 °C: 24.5 l/mol
1 liter of oxygen is \( \frac{1}{24.5} = 0.0408 \) mol
Conversion to mass: \( 0.0408 \times 32 = 1.31 \) g

Stoichiometric calculations

Example: In the reaction between barium nitrate and sodium sulfate, how many grams of barium sulfate can be prepared from 10 ml of 10% (w/v) barium nitrate? Take into account that about 5% of the product is lost.
(AW of barium: 137.3, sulfur: 32.1, nitrogen: 14.0, oxygen: 16.0)

\[
\text{equation: } \text{Ba(NO}_3\text{)}_2 + \text{Na}_2\text{SO}_4 \rightarrow \text{BaSO}_4 + 2\text{NaNO}_3
\]

FW Ba(NO\(_3\)\(_2\): 261.3  
FW BaSO\(_4\): 233.4

10 ml of 10% (w/v) Ba(NO\(_3\)\(_2\): 1 g .. \( \frac{1}{261.3} = 0.003827 \) moles

amount of BaSO\(_4\) formed: \( 0.003827 \) moles ....

... \( 0.003827 \times 233.4 = 0.8932 \) g (theoretical yield, 100%)

Actual yield: \( 0.8932 \times 0.95 = 0.849 \) g
Stoichiometric calculations

Equation coefficients

1. Mol/l of A
2. Grams of A
3. Grams/l of A
4. Liters of A (if gas)
5. Moles of A

6. Mol/l of B
7. Grams of B
8. Grams/l of B
9. Liters of B (if gas)
10. Moles of B

Stoichiometric calculations

Theoretical yield (100%)

Actual yield

Loss