Quantitative chemistry
(quantity calculus)

Practical info

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- Textbook: Bettelheim, Brown, Campbell, Farrell “Introduction to general organic and biochemistry” EdiSES
- Any other general and organic chemistry book with solved exercises

Weights and measures

- A physical quantity is the product of a numerical value and a unit of measurements

- On the importance of units of measurements:

  1000 → this is just a number
  1000 lb → this is the weight of some goods
  1000 kg → this is a weight too, but the quantities are not the same

- International System of Units (SI): the modern form of the metric system

Unit name	**Unit symbol**	**Quantity name**
metre	m	length
kilogram	kg	mass
second	s	time
liter	*L* or *l*	volume
kelvin	K	thermodynamic temperature
mole	mol	amount of substance

Weights and measures

- Standard prefixes to vary quantities in the SI

Multiples	**Name**		deca-	hecto-	kilo-	mega-	giga-	tera-	peta-	exa-	zetta-	yotta-
	Symbol		da	h	k	M	G	T	P	E	Z	Y
	Factor	10^0	10^1	10^2	10^3	10^6	10^9	10^{12}	10^{15}	10^{18}	10^{21}	10^{24}
Fractions	**Name**		deci-	centi-	milli-	micro-	nano-	pico-	femto-	atto-	zepto-	yocto-
	Symbol		d	c	m	µ	n	p	f	a	z	y
	Factor	10^0	10^{-1}	10^{-2}	10^{-3}	10^{-6}	10^{-9}	10^{-12}	10^{-15}	10^{-18}	10^{-21}	10^{-24}

Why do we need quantity calculus in both laboratory and wards?

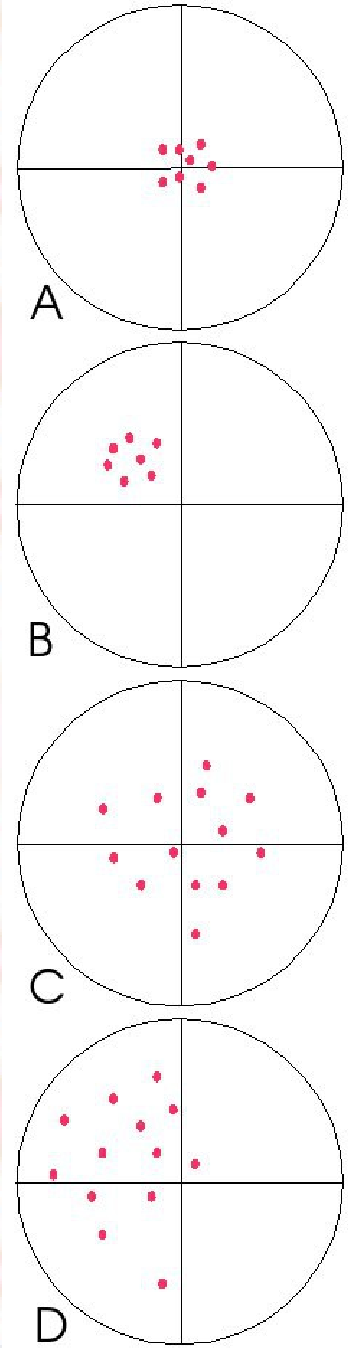
- Data collection → we need to experimentally measure some parameters (e.g. urine colour)
- Data analysis → we need to convert a given parameter into another one (e.g. from urine colour to concentration)
- Results → we need to compare the actual concentra tion to physiological values before infer ring a diagnosis

Experimental errors and significant digits

- All experimental measurements are affected by errors, which we ought to keep to a minimum
- Any experimental measurement needs to be both accurate and precise

Accuracy → the measured value needs to be as close as possible to the real value

Precision → reproducibility of measurements (how close are the measured quantities with one another)



A: accurate and precise measures
B: precise but NOT accurate measures
C: accurate but NOT precise measures
D: measures neither accurate nor precise

Experimental errors and significant digits

- Within a given experiment accuracy and precision are both needed to determine the amount of significant digits of the result numbers

- Example: we are measuring the volume of a box; we repeat each measure 4 times; here are the values we obtained:
  - 1^{st} measure: 52.8 *l*
  - 2^{nd} measure: 52.6 *l*
  - 3^{rd} measure: 52.9 *l*
  - 4^{th} measure: 52.5 *l*

The average value is:

$$\Sigma(\text{measures})/\text{no.measures} = 52.8+52.6+52.9+52.5)/4 = = 52.7\ l$$

How precise is this average no.?

- Let's calculate the single deviations with the formula: $d_i=(n_i-<n>)$
- Let's calculate the average of the deviations:

$$\Sigma|d_i|/i = (0.1+0.1+0.2+0.2)/4=0.15\ l$$

The volume of the box is 52.70 ± 0.15 *l*

Experimental errors and significant digits

- The error on the final number has to be as close as possible to the intrinsic error of the instrument
- When we need to sum parameters, the final result cannot be more precise of the least precise quantity (e.g. the significant digits cannot be more than those pertaining to the least precise no.)

ex.: 25.362 m + 121.38 m = 146.74 m NOT 146.742 m

In quantitative calculus numbers cannot be always considered in the same way. In fact there are:

Parameters → measurable quantities, hence affected by errors

Constants → numbers whose significant digits need to be ALWAYS considered in full (ex. Avogadro constant: $N_A = 6.022 \times 10^{23}$)

Let's practice

How many grams are in 1 Kg?	1000 g = 10^3 g
How many milligrams are in 1Kg?	10^6 mg
How many grams correspond to 1000 mg?	1 g
How many Kg correspond to 10^2 g?	0.1 Kg
How many grams are there in 10^{-3} Kg?	1 g
How many ml are in 1L?	1000 ml = 10^3 ml
How many sec are in 10 minutes?	600 s

It is convenient to use the power of ten as exponentials

- Example:

Instead of 0.0001: use 10^{-4}
Instead of 10000: use 10^{4}

Convert the following numbers in exponentials:

◆ 378000	3.87×10^{5}
◆ 8931.5	8.93×10^{3}
◆ 0.000593	5.93×10^{-4}
◆ 0.000004	4.0×10^{-6}

Elements and Molecules

- Elements (atoms): the smallest unit of a compound/particle
- Atomic symbol: acronym composed by 1 or 2 letters, unequivocally indicates the element
- Periodic table (Mendeleyev table): classification of atoms based on the atomic number and on physical-chemical characteristics

$$^{A}_{Z}X^{C}_{*}$$

- A is the mass number: no. protons + no. neutrons
- Z is the atomic number: either no. of protons or no. electrons
- C is the atomic charge (0=neutral; +i=cation; -i=anion)
- * is the number of that atom in a molecular brute formula

- Isotopes: atoms with the same Z, but different A

Useful Units for the Atoms/Molecules

- *Mole*: a quantity comprising a $N_{Avogadro}$ of atoms/molecules (6.022×10^{23})
- *Atomic mass units* (AMU or Da): 1.67×10^{-24} g = 1/12 of the mass of ^{12}C
- *Relative atomic mass* (RAM): mass of each atom referred in AMU, relative mass of an atom with respect to 1/12 of ^{12}C
- *Relative molecular mass (Formula weight, FW)*: is the sum of the atomic masses of the single atoms in a compound

Ex.:

Which is the RAM of Oxygen?	16 Da
Which is the RAM of Nitrogen?	14 Da
Which is the FW of water (H_2O)?	1+1+16=18 Da
Which is the FW of carbonic acid (H_2CO_3)?	1+1+12+16+16+16=62 Da

Which is the relationship between MOLE and MASS?

- 1 *mole* of a given atom/compound = quantity in *g* of the mass of that atom/compound

$$n \text{ (mol)} = \text{mass (g)} / \text{FW (Da)}$$

How many *mol* correspond to 5g of CO_2?

FW = 12 +16+16 = 44 Da ($gmol^{-1}$)

$n = \text{mass}/\text{FW} = 5g/44gmol^{-1} = 0.11$ mol

Exercise 1

How many moles correspond to 100g of ethanoic acid, aka acetic acid (CH_3COOH)?

FW= (2x12) + (4x1) + (2x16) = 60

n= mass/FW = 100/60 = 1.67 mol

Exercise 2

How many grams correspond to 22 mol carbon dioxide (CO_2)?

FW= (1x12) + (2x16) = 44

n= mass/FW hence mass= n x FW

mass= 22 x 44 = 968g

Exercise 3

5mg of a drug are contained in 10 ml of a solution. How many ml do we need to infuse to a patient, given that the needed dose is 2mg? How many grams of drug are in 0.05 *l* of this same solution?

$5mg:10ml = 2mg: x_1$

$x_1 = (10ml \times 2mg) / 5mg = 4ml$

$0.05l = 0.05 \times 1000\ ml = 50ml$

$5mg:10ml = x_2:50ml$

$x_2 = (5mg \times 50ml)/10ml = 25mg$

The Gas phase:
Ideal gases

Characteristics of ideal gases

- An ideal gas is a theoretical gas made by
  - Point particles (very very very very small volume)
  - Randomly and fast moving particles
  - Not interacting particles
- The particles have a constant energy which is preserved after colliding against both other particles and the container's walls
- At normal conditions such as standard temperature and pressure, most real gases (i.e. air, O_2, N_2, He, Xe) behave qualitatively like an ideal gas

Thermodynamics laws of ideal gases

- Isothermal law (aka Boyle's law) T=constant
  $PV=k_1$
- Isobaric law (aka Charles' law) P=const.
  $V=k_2T$
- Isochoric (isovolumetric) law (aka Gay-Lussac's law) V=const.
  $P=k_3T$
- Avogadro's law: two given samples of an ideal gas, at the same temperature, pressure and volume, contain the same number of particles.
  $$\frac{V}{n}=k4$$
  V= molar volume = 22.4 *l* at 273K and 1 atm

Combined gas law

- The combined gas law combines the 4 aforementioned laws and states that:

"The ratio between the pressure-volume product and the temperature of a system remains constant"

$$PV = nRT$$

Where P is measured in atm; V in litres; T in K; and R is the universal gas constant, whose number depends on the digital units employed

R= 0.082 *l* atm mol^{-1} K^{-1}

R= 1.987 *cal* mol^{-1} K^{-1}

R= 8.314 J mol^{-1} K^{-1}

Exercise 4

- Which is the pressure applied by 16g of molecular oxygen (O_2) in a cylinder of 25 *l* at 18°C?

Which is the unknown quantity?

Pressure → let's apply the combined gas law PV=*n*RT

n= g/FW = 16/32 =0.5 mol
T = t(°C)+273 = 18+273 = 291K

$$P=\frac{nRT}{V}=\frac{0.5\,mol\,x\,0.082\,l\,atm\,x\,291\,K}{25\,l\,mol\,K}=0.48\,atm$$

Exercise 5

In a cylinder of 2 *l*, connected to a vacuum pump, the residual gas pressure is $3.0 \cdot 10^{-6}$ mmHg at 20°C. How many molecules are left?

Which is the unknown quantity? *n*

We need to convert units before applying the combined gas law:

T=20+273 = 293K
P= $3.0 \cdot 10^{-6}/760 = 3.95 \cdot 10^{-9}$ atm

$$n = \frac{PV}{RT} = \frac{3.95\text{x}10^{-9}\, atm * 2\, l * mol\, K}{0.082\, l\, atm * 293\, K} = 3.29\text{x}10^{-10}\, mol$$

Avogadro's law states that there are $6.022 \cdot 10^{23}$ molecule in 1 mol, hence:
no.molecules= N*n = $6.022 \cdot 10^{23} \cdot 3.29\ 10^{-10} = 1.98 \cdot 10^{14}$

Exercise 6

- At which temperature, expressed in Celsius units, 2g of dioxygen fill in a volume of 1.5 *l* at 5 atm pressure?

We need to calculate T

n=g/FW=2/32 = 0.0625 mol

$$T = \frac{PV}{nR} = \frac{5\,atm * 1.5\,l\,mol\,K}{0.0625\,mol * 0.082\,l\,atm} = 1463\,K$$

T(°C) = 1463K - 273 = 1190°C

Exercise 7

- 0.66 g of an unknown gas are filling in a volume of 200 ml at 1368 mmHg and at 20°C. Calculate the gas's FW.

Let's start converting:

V= 200ml/1000 = 0.2 *l*

P= 1368 / 760 = 1.8 atm

T = 20+273 = 293 K

n= g/FW → let's modify the combined gas law: $n=\frac{PV}{RT} \rightarrow \frac{g}{FW}=\frac{PV}{RT}$

$$FW=\frac{gRT}{PV}=\frac{0.66*0.082*293}{1.8*0.21}=44.05$$

Exercise 8

- Given a cylinder of 5.6 *l* at 0°C and 1 atm, which of the following gas is going to fill in it?
  - a) 14 g of molecular nitrogen
  - b) 16 g of dioxygen
  - c) 5 g of Neon ok
  - d) 32 g of dioxygen

The unknown quantity is n → n= PV/RT = (1*5.6)/(0.082*273)= 0.25 mol

a) n= g/FW= 14/28 = 0.5 mol
b) n= 0.5 mol
c) n= 0.25 mol
d) n= 1 mol

Exercise 9

- A certain amount of gas is filling in a volume of 350 ml at 150°C and 0.7 atm. Calculate the pressure which the same gas is going to have in a volume of 2 *l* at 30°C.

The gas is undergoing a transformation from state1 (P1, T1, V1) to state2 (P2, T2, V2): which quantity does remain constant?

The number of mole, hence we can rearrange the combined gas law as follows:

$$\frac{P_1 * V_1}{T_1} = \frac{P_2 * V_2}{T_2}$$

$$P_2 = \frac{P_1 * V_1 * T_2}{T_1} * V_2 = \frac{\{0.7\,atm * 0.35\,l * 303\text{K}\}}{\{423\,K * 2\,l\}} = 8.77\text{x}10^{-2}\,atm$$

Exercise 10

- A certain quantity of gas is inside a cylinder, closed by a piston, at 308K. It is heated, under constant pressure, up to a point in which the final volume is twice the initial one. Which is the final temperature in degree celsius?

P= constant; n= constant;
hence the combined gas law is simplified as such: $\frac{V_1}{T_1}=\frac{V_2}{T_2}$

$$T_2=\frac{V_2 * T_1}{V_1}=\frac{2V_1 * T_1}{V_1}=2T_1$$

T_2= $2T_1$ = 2x308 K = 616K = 616-273 = 343°C