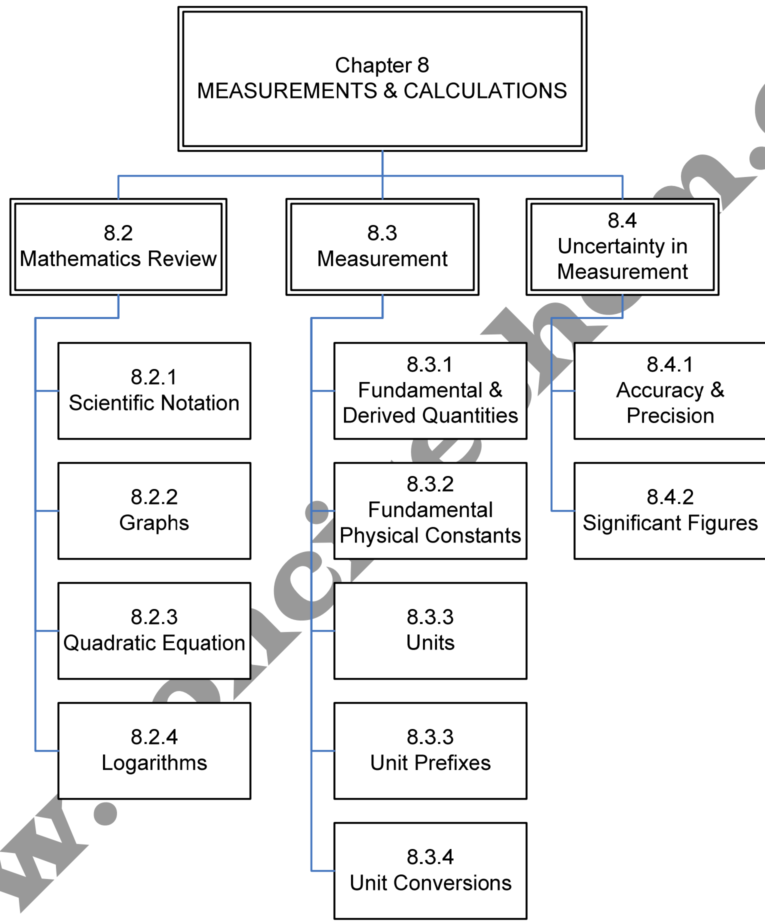
Chapter 8

Measurements & Calculations

This is where an introduction to every chapter goes. Make it very brief..

8.1 Chapter Concept Map



8.2 Mathematics Review

Knowledge of basic mathematics is a prerequisite for solving computational problems in chemistry. Sections below summarize the essentials.

<u>Inquisitive Chemist 8.1</u>: Useful resources

Equations in Chemistry
http://www.mhhe.com/physsci/chemistry/chang7/esp/tools/equations/equations.htm (McGraw Hill)

Unit conversions
http://www.chemie.fu-berlin.de/chemistry/general/units_en.html

8.2.1 Scientific Notation

Scientific notation provides a compact and convenient way of writing very large and very small numbers. This is done by simply expressing the number as the product of a number between 1 and 10, times the number 10 raised to a power. See examples below which cover the four possible combinations.

<u>Sample Problem 8.1</u>: Express numbers in scientific notation.

Questions
1. 56897
2. 0.00023

Answers
1. Number needs to be expressed as a product of number between 1 & 10 raised to a power $\Rightarrow 5.6897 \times 10^y \Rightarrow y = 4$ because the decimal point needs to be moved to the right by 4 decimal places; i.e. positive exponent makes the number larger.
2. Number needs to be expressed as a product of number between 1 & 10 raised to a power $\Rightarrow 2.3 \times 10^y \Rightarrow y = -4$ because the decimal point need to be moved to the left by 4 decimal places; i.e. negative exponent makes the number smaller.

<u>Sample Problem 8.2</u>: Express following numbers in decimal notation.

Questions
1. 4.123×10^2
2. 5.73×10^{-5}

Answers
1. Positive exponent $\Rightarrow$ makes the number larger $\Rightarrow$ move decimal to the right $\Rightarrow$ 412.3
2. Negative exponent $\Rightarrow$ makes the number smaller $\Rightarrow$ move decimal to the left $\Rightarrow$ 0.0000573

Addition & Subtraction

To add or subtract numbers expressed in scientific notation, all numbers must have the same exponent.

Multiplication & Division
- To multiply: $(A \times 10^y)\ (B \times 10^x) = (A \times B)\ (10^{y+x})$.
- To divide: $(A \times 10^y) \div (B \times 10^x) = (A \div B)\ (10^{y-x})$.
- Exponents: $(A \times 10^y)^z = A^z \times 10^{y \cdot z}$
- Root: $\sqrt[z]{A \times 10^y} = (A \times 10^y)^{1/z} = A^{1/z} \times 10^{y/z}$

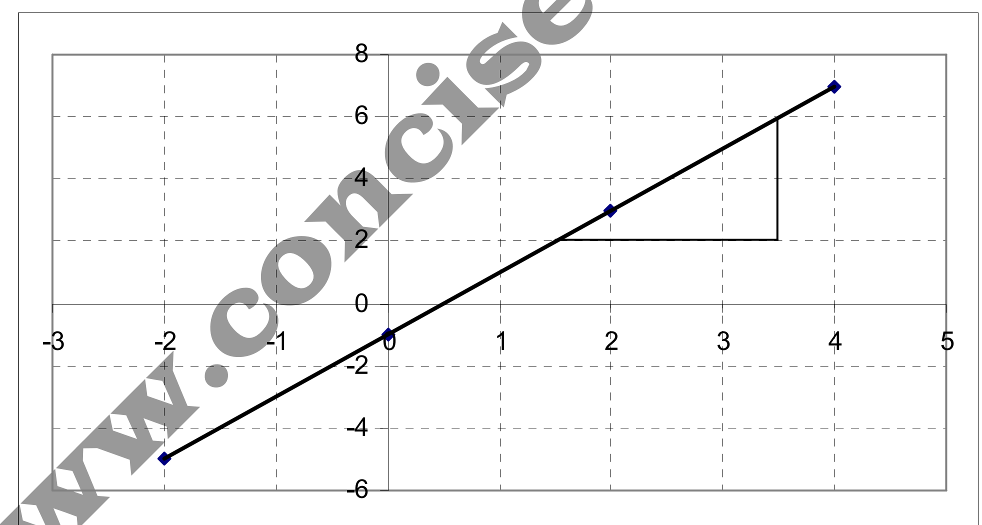
Sample practice problems on scientific notation and calculations can be found at http://www.edinformatics.com/math_science/scinot.htm.

Calculators
Calculator is your best friend when it comes to calculations. Chemistry uses a lot of really big and small numbers, so make sure you know how use your calculator to solve scientific notation problems. If you don't have one, do yourself a big favor and buy a scientific calculator today and learn how to use it.

8.2.2 Graphs

In chemistry, you'll come across many graphs. Let's consider an example below.

Figure 8.1: Reading a Graph



Things you should know:
- X is always the horizontal axis and is the **independent variable**.
- Y is the vertical axis and is a **dependent variable** (i.e. it depends on the value of x).
- Experimental values are plotted as dots on the graph and connected by a straight line.
- This is a straight line plot, which means that we can write an equation for it in the form

$$y = mx + b$$

where

y	=	y value
x	=	x value

m	=	slope = $\frac{\Delta y}{\Delta x}$
b	=	intercept

- The right triangle in above graph show that y changes from 2 to 6 ($\Delta y = 4$) when x changes from 1.5 to 3.5 ($\Delta x = 2$). Therefore, the **slope** of the line is 2.
- The y intercept is -1, hence b = -1.
- The **linear equation** is therefore: *y = 2x-1*

8.2.3 Quadratic Equation

The only topic that will involve calculations with the quadratic equation is chapter 12 (kinetics of reactions). The **quadratic equation** can be written as

$$ax^2 + bx + c = 0$$

where

a	=	constant
b	=	constant
c	=	constant

Notice that the only variable in the equation is x. The 2 solutions for the quadratic equation are given by the **quadratic formula**

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

where

a	=	constant
b	=	constant
c	=	constant

8.2.4 Logarithms

You'll encounter logarithms mostly with problems dealing with acids and bases (chapters 18 & 19). This is another area where the scientific calculator will become very hand so make sure to familiarize yourself with the log functions on your calculator.

Common Logarithm (or simply logarithms or **log**)
All positive numbers (let's call them x) can be written in terms of 10^y. Exponent y is the base 10 logarithm of x and can be written as $\log_{10}x$ or simply log x. That is

$$x = 10^y \text{ or } \log x = y$$

where

x	=	any positive number

For example, log of 1000 is 3 because $1000 = 10^3$. So essentially, the log of a number x is the power y to which 10 must be raised.

General observations about logarithms:
- When x > 1, log x = +
- When x = 1, log x = 0
- When 0 < x < 1, log x = -
- When $x \leq 0$, log x = undefined because 10 raised to any number is always positive.

Antilogarithm (or simply **antilog**)
Antilogarithm is the inverse of a logarithm. Going back to the above example where log x = y, we can say that antilog of y = x. So essentially, the antilog of a number x is 10 raised to power x.

Natural Logarithm (or simply **ln**)
Natural logarithm is the same as common logarithm, except that base 10 is substituted with *e* (= 2.71828).

$$x = e^y \text{ or } \ln x = y$$

where

x	=	any positive number
e	=	2.71828

If we were to manipulate equations a bit, we would arrive to the following

$$\ln x = 2.303 (\log x)$$

where

x	=	any positive number

Mathematical Manipulations of Logarithms (only log shown but also true for ln)

- $\log x{\cdot}y = \log x + \log y$
- $\log x/y = \log x - \log y$
- $\log x/y = - \log y/x$
- $\log 1/x = - \log x$
- $\log x^a = a (\log x)$

Sample Problem 8.3: Calculate the logarithm and antilogarithm.

Questions

1. What is the log of 100?
2. What is the antilog of 100?
3. What is the ln of 100?

Answers

1. 100 can be written as $10^2 \Rightarrow$ log of 100 is 2.
2. 10^{100}.
3. 100 can be written as $e^y \Rightarrow$ y = 4.60 (using a calculator); or ln x = 2.30 (log x) $\Rightarrow$ ln x = 2.30 · (2) = 4.60

Section Test

Questions

1. Which is greater: 6.0×10^6 or 2.0×10^3? How many times?
2. What is the log of 53.2?

Answers

1. 6.0×10^6 is 3000 times greater.
2. Using your calculator, press 53.2 and then "log" $\Rightarrow$ 1.73. You know that the answer should be between 1 & 2 because 53.2 is between 10^1 & 10^2.

8.3 Measurement

If I were to ask you how much you weight and you told me 150, I really wouldn't know how much you weight. Why – because telling me simply 150 doesn't tell me if your balance measures in lbs or kgs. Measured quantity must have both a number and a unit for the measurement to have any meaning.

8.3.1 Fundamental & Derived Quantities

There are seven **fundamental quantities.**

- **Mass**: measure of quantity of matter.
- **Length**: measure of distance or dimension.
- **Temperature**: measure of hot or cold something is, and determines direction of **heat** flow. Heat is the *energy that is transferred between objects* caused by differences in their temperatures.
- **Time**: measure of period when something occurs.
- **Electric current**: measure of flow of electric charge.
- **Amount of substance**: measure of amount of substance in terms of a mole. Mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kilogram of ^{12}C.
- **Luminous intensity**: measure of the wavelength-weighted power emitted by a light source in a particular direction; not used in chemistry.

Derived quantities are physical quantities made by combination of fundamental quantities. For example, volume is a derived quantity obtained from 3 length measurements.

8.3.2 Fundamental Physical Constants

Fundamental physical constants play a fundamental role in physics and chemistry. You have encountered some in chapter 3 (e.g. mass of electron, m_e; Planck's constant, h) and will encounter many more in the formulas of the upcoming chapters. Table below shows the constants that you will use in this course. Do not memorize them because they will be given to you on the exam; simply learn how to use them in calculations. An exhaustive list of constants is available (pdf or html) at http://physics.nist.gov/constants, which is maintained by Committee on Data for Science and Technology (CODATA) of National Institute of Standards and Technology (NIST). In you calculations for the class, you'll use this numbers approximated at the second or third decimal place.

Table 8.1: Most Commonly Used Fundamental Physical Constants

Quantity	Symbol	Value	Unit
Absolute Temperature	T_0	273.15	K
Atomic Mass Unit	m_u	$1.66053873(13) \times 10^{-27}$	kg
Avogadro's Number	N_A	$6.02214199(47) \times 10^{23}$	mol^{-1}
Bohr Magneton	μ_B	$9.27400899(37) \times 10^{-24}$	$J{\cdot}T^{-1}$
Bohr Radius	a_o	$0.5291772083(19) \times 10^{-10}$	m
Boltzmann's Constant	k	$1.3806503(24) \times 10^{-23}$	$J{\cdot}K^{-1}$
Deuteron Mass	m_d	$3.34358309(26) \times 10^{-27}$	kg

Electric Constant	ε_o	$8.854187817 \times 10^{-12}$	$F \cdot m^{-1}$
Electron Mass	m_e	$9.10938188(72) \times 10^{-31}$	kg
Electron-Volt	eV	$1.602176462(63) \times 10^{-19}$	J
Elementary (Electron) Charge	e	$1.602176462(63) \times 10^{-19}$	C
Faraday Constant	F	$9.64853415(39) \times 10^{4}$	$C \cdot mol^{-1}$
Fine Structure Constant	α	$7.297352533(27) \times 10^{-3}$	
Hydrogen Ground State		13.6057	eV
Magnetic Constant	μ_o	$4\pi \times 10^{-7}$	
Molar Gas Constant	R	8.314472(15) 0.0820574 1.987 62.36	$J \cdot K^{-1} \cdot mol^{-1}$ $L \cdot atm \cdot K^{-1} \cdot mol^{-1}$ $cal \cdot K^{-1} \cdot mol^{-1}$ $L \cdot torr \cdot mol^{-1} \cdot K^{-1}$
Newtonian Constant of Gravitation	G	$6.673(10) \times 10^{-11}$	$m^3 \cdot kg^{-1} \cdot s^{-2}$
Neutron Mass	m_n	$1.67492716(13) \times 10^{-27}$	kg
Nuclear Magneton	μ_n	$5.05078317(20) \times 10^{-27}$	$J \cdot T^{-1}$
Pi	π	3.1415927	
Planck Constant	h	$6.62606876(52) \times 10^{-34}$	$J \cdot s$
Planck Length	l_p	$1.6160(12) \times 10^{-35}$	m
Planck Mass	m_p	$2.1767(16) \times 10^{-8}$	kg
Planck Time	t_p	$5.3906(40) \times 10^{-44}$	s
Proton Mass	m_P	$1.67262158(13) \times 10^{-27}$	kg
Rydberg Constant	R_H	$10\ 9.73731568549(83) \times 10^{5}$	m^{-1}
Speed of Light in Vacuum	c	2.99792458×10^{8}	$m \cdot s^{-1}$

* Values given below are from the CODATA 2002 recommended by NIST
* Values contain uncertainty in the last two decimal places given in brackets. Values that do not have this uncertainty listed are exact.

Inquisitive Chemist 8.1: Additional resource on constants.

Barrow. The Constants of Nature; From Alpha to Omega - The Numbers that Encode the Deepest Secrets of the Universe. Pantheon Books, 2002.

8.3.3 Units

Base Units

Metric and International System of Units (SI) are most commonly used systems in designating units, although the SI is internationally recognized as the official system of units. The British units are not used in scientific measurements. In fact, many countries using the British system have made the switch to the metric system or are in the process of doing so. Table below summarized the units for the seven fundamental quantities, and shows some equivalents used in calculations and for your reference. Complete list of SI units can be viewed at http://physics.nist.gov/cuu/Units/units.html.

Table 8.2: Base Units

Quantity	Metric Unit	SI Unit	SI Name	Equivalent
Mass	g	kg	kilogram	kg = 2.2 lbs; ton = 1,000 kg
Length	m	m	meter	m = 3.3 ft; A (angstrom) = 10^{-10} m; mile = 1.61 km
Temperature	°C	K	Kelvin	K = 273.15 + °C; °C = K - 273.15 °F = 9/5·(°C) + 32; °C = 5/9·(°F-32)
Time	s	s	second	
Electric Current	A	A	ampere	
Amount of Substance	mol	mol	mole	mol = 6.02×10^{23} particles

Luminous Intensity	cd	cd	candela

Derived Units

All other units that you will encounter are derived units. Some might even have special names for convenience, but you should always know what base units they're derived from. For example, volume is a derived quantity and is measured with a derived unit of liters (L). In base units, 1L is 1,000 cm^3. Other derived units that you will use in chemistry are summarized in the table below.

Table 8.3: Derived Units Used in Chemistry

Quantity	SI Name	SI Symbol	SI Base Units Equivalent	Other Equivalent
Absorbed Dose	gray	Gy	$m^2 \cdot s^{-2}$	Gy = J/kg; rad = 10^{-2} Gy
Activity (of a radionuclide)	becquerel	Bq	s^{-1}	Ci = 3.7×10^{10} Bq
Area			m^2	
Capacitance	farad	F	$m^{-2} \cdot kg^{-1} \cdot s^4 \cdot A^2$	F = C/V
Dose Equivalent	sievert	Sv	$m^2 \cdot s^{-2}$	Sv = J/kg; rem = 10^{-2} Sv
Electric Charge	coulomb	C	$s \cdot A$	
Electric Potential	volt	V	$m^2 \cdot kg \cdot s^{-3} \cdot A^{-1}$	V = W/A
Energy; Work: Heat	joule	J	$m^2 \cdot kg \cdot s^{-2}$	J = N·m; cal = 4.184 J
Entropy		J/K	$m^2 \cdot kg \cdot s^{-2} \cdot K^{-1}$	
Exposure	C/kg		$kg^{-1} \cdot s \cdot A$	
Force	newton	N	$m \cdot kg \cdot s^{-2}$	
Frequency	hertz	Hz	s^{-1}	
Heat Capacity		J/K	$m^2 \cdot kg \cdot s^{-2} \cdot K^{-1}$	
Molar Energy		J/mol	$m^2 \cdot kg \cdot s^{-2} \cdot mol^{-1}$	
Molar Heat Capacity		J/(mol·K)	$m^2 \cdot kg \cdot s^{-2} \cdot mol^{-1} \cdot K^{-1}$	
Power	watt	W	$m^2 \cdot kg \cdot s^{-3}$	W = J/s
Pressure	pascal	Pa	$m^{-1} kg \cdot s^{-2}$	Pa = N/m^2; atm = 760 torr = 760 mmHg = 101,325 Pa; bar = 10^5 Pa
Specific Heat Capacity		J/(kg·K)	$m^2 \cdot s^{-2} \cdot K^{-1}$	
Speed			m/s	
Volume			m^3	quart = 0.946 L; 3.785 L = gal; L = dm^3 = 10^{-3} m^3
Wave Number			m^{-1}	

8.3.4 Unit Prefixes

Prefixes in both the Metric and SI systems are used as decimal multiples of the base unit. They can either make the base unit larger or smaller. Prefixes are summarized in the table below.

Table 8.4: Unit Prefixes

Prefixes that INCREASE base units			Prefixes that DECREASE base units		
Factor	**Prefix**	**Symbol**	**Factor**	**Prefix**	**Symbol**
10^1	deka	da	10^{-1}	deci	d
10^2	hecto	h	10^{-2}	centi	c
10^3	kilo	k	10^{-3}	milli	m
10^6	mega	M	10^{-6}	micro	μ

10^{9}	giga	G	10^{-9}	nano	n
10^{12}	tera	T	10^{-12}	pico	p
10^{15}	peta	P	10^{-15}	femto	f
10^{18}	exa	E	10^{-18}	atto	a
10^{21}	zeta	Z	10^{-21}	zepto	z
10^{24}	yotta	Y	10^{-24}	yocto	y

Sample Problem 8.4: Our universe is comprised of vast size ranges. For example, size of the observable universe is estimated to be 10^{28} cm, diameter of Earth is 10^{9} cm, and diameter of an atomic nucleus is 10^{-13} cm. How many times is the universe larger than Earth? How many times is the universe larger than the atomic nucleus?

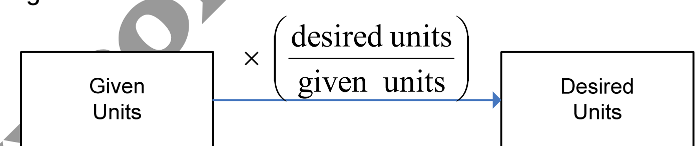
Universe is 10^{19} times larger than Earth and 10^{41} times larger than the atomic nucleus.

Inquisitive Chemist 8.2: Attosecond Spectroscopy.

Attosecond spectroscopy is one example where chemists use really small units in their measurements. Until recently, the technology for the motion at atomic levels was limited to the duration of a single cycle of visible light (i.e., 1 femtosecond), which was not precise enough to probe motions of electrons. In the last few years, however, laser technology has enabled scientists to measure at the attosecond level which is precise enough to track electron rearrangements in chemical bonding. More information can be found at http://www.attoworld.de/index.html.

8.3.5 Unit Conversions

Unit conversion approach is a series of multiplications of conversion factors that affords an easy route to changing the units of measurement from one unit to another similar unit.



Conversion factor simply expresses numerical relationships between units as a proportion that is always equal to one. All we're doing is multiplying by 1. For example, if we want to change number 32 to a fraction with a five denominator, we simply multiply by 1 (i.e. 5/5) $\Rightarrow 32 \times 1 = 32 \Rightarrow 32 \times 5/5 = 160/5$.

Sample Problem 8.5: It takes you 48 seconds to read one page of the book. How many seconds will it take you to read a 300 page book? Minutes? Hours?

$$\frac{48\text{ s}}{1\text{ pg}} \times 300\text{ pg} = 14{,}400\text{ s} \times \frac{1\text{ min}}{60\text{ s}} = 240\text{ min} \times \frac{1\text{ hr}}{60\text{ min}} = 4\text{ hrs}$$

In summary, when converting from one unit to another, always follow the three step process:

- What data are we given?
- What units do we need?
- What conversion factors will get us from units we are given to units that we need?

<u>Sample Problem 8.6</u>: Patient requires injection of 0.012g of pain killer available as a 15mg/mL solution. How many mL should be administered?

The problem is asking to calculate mL from g. We can do that by $g \times \left(\frac{mL}{g}\right) = mL$

Hence $0.012g \times \left(\frac{1\,mL}{.015g}\right) = 0.80mL$

<u>Section Test</u>

Questions

1. Convert 30 ng to kg.
2. Covert 293 K to °F.
3. You're driving in Canada, and notice the speed sign of 100. You press on the pedal and speed off just to be pulled over by police and ticketed for speeding. Why did you get pulled over? What was the speed limit in miles?

Answers

1. $30\ ng \Rightarrow 3.0 \times 10^{-9}\ g \Rightarrow 3.0 \times 10^{-12}\ kg$
2. 68 °F
3. $$100\ km \times \left(\frac{0.62\ miles}{1\ km}\right) = 62\ miles$$

8.4 Uncertainty in Measurement

All measurements have some uncertainty or error associated with them. For example, when you measure your weight on the home balance (balance A), it gives you the weight in kgs; there's no way to know certainly how many grams beyond the kg are also there. Similarly, when you're in a lab, you can measure weights to the nearest 1/100 of a gram (balance B), but don't know much beyond that. If you work in an analytical lab, you would have the capacity to measure to the nearest 1/10,000 g (balance C). In all cases (balances A, B & C), there was some uncertainty.

<u>Inquisitive Chemist 8.2</u>: Additional resource on how science deals with uncertainty.

Pollack. Uncertain Science, Uncertain World. Cambridge University Press: Cambridge, 2003.

8.4.1 Accuracy & Precision

We say that all measurements are inexact. This can be due to **mistakes** (carelessness) while making measurements, and/or due to inherent limitations in the measurement (limitations in instruments and/or methods).

- **Systematic errors** are *variations in just one direction*.
- **Statistical (random) errors** are *positive & negative deviations* from true value.

Inquisitive Chemist 8.3: Science methods can get quite complex.

Click on the links below to see some methods developed by U.S. EPA and OECD.
http://www.epa.gov/epahome/index/sources.htm
http://www.oecd.org/document/22/0,3343,en_2649_34377_1916054_1_1_1_1,00.html

Accuracy

Accuracy refers to the *proximity of a measurement to the true value* of a quantity (correctness of measurement). Calibration (fine tuning) can eliminate errors that affect accuracy.

Precision

Precision refers to the *proximity of several measurements to each other*. Precisions errors are due to random errors (or **noise**), and can be minimized by averaging values over a large number of measurements.

Sample Problem 8.7: You're given an object whose real mass is 1.233 g, and told to obtain two weight readings from three balances. You measure the following weights: balance 1 (1.233 g, 1.234); balance 2 (1.134 g, 1.135 g); balance 3 (1.025 g, 1.179 g). Which of these balances gave precise measurements? How about accurate measurements? What kind of error (systematic or random) error do we see with balance 2?

Balances 1 & 2 gave precise (reproducible) measurements. Balance 1 gave accurate measurements. Balance 3 gave inaccurate and imprecise readings. Readings from balance 2 are precise but not accurate, suggesting that we have systematic errors (need to recalibrate the instrument and/or look at the test method).

8.4.2 Significant Figures

Suppose we weight a penny coin on the three balances mentioned above, and got the following readings:

- Balance A: 0 kg
- Balance B: 2.60 g
- Balance C: 2.60000 g

Which one would you prefer? Obviously balance C, but is balance C telling us anything more than balance B? Answer is yes – more digits that we have in the measurement, more reliable are the data. In balance B we weren't sure about the digit x in 2.60x, but with balance C we knew that x in 2.60x is 0. We say that the last digit (most to the right) has some uncertainty in it because we don't know the number that follows it and hence it's only estimated (rounded up or down).

Significant figures (digits) are number *of meaningful digits used to express a value*.

- Measuring devices: all digits obtained + first approximated digit are significant
- Digital devices: all digits obtained are significant (no way to approximate next digit)

Tables 8.1 and 8.2 below summarize rules for recognizing significant figures and for using them in calculations.

Table 8.5: Postulates for Recognizing Significant Figures

Postulate	Example	Number of Significant Figures
All nonzero numbers are significant.	3569	4
Zeros before a decimal are not significant. They are placed there as a formality to enhance the view of the decimal point.	0.23	2
Zeros between significant digits are significant.	2003	4
Zeros used to indicate precision (to the right of decimal and significant digits) are significant.	14.00 0.760	4 3
Placeholder zeros are not significant.	0.05 300	1 1
All digits in the nonexponential (front) portion of a scientific notation are significant.	1.20×10^5 3.6×10^{-2}	3 2
Numbers which are "exact" (such as many conversion factors) have an infinite (∞) number of significant figures.	100 cm in 1m 32 students in class	∞ ∞
When taking logarithms (such as pH) the number of digits to the right of the decimal in the log is equal to the number of significant figures in the value which the log is taken of.	-log 0.012	3 Answer would be expressed as 1.92

Table 8.6: Rules Involving Calculations

Function	Rule	Example	Answer
Multiplication & Division	The answer must be rounded off to the number of significant figures which are the same as that of the *least significant* digit value used in calculation.	(0.0348) x (2.1) 0.01 ÷ 0.62	0.073 0.02
Addition & Subtraction	The precision (places) of the answer must be the same as the *least precise* number used in the calculations.	23.6 + 41 41 – 23.6 8.4 + 7.8 0.788 – 0.77	65 17 16.2[a] 0.02[b]
Average	The average result must contain the *same precision* as the component values being averaged.	98.6, 99.0, 98.4	98.7
Logarithms	The only significant figures are the digits to the right of the decimal point; numbers on the left are just place holders.	log 53.2 log 53	1.726[c] 1.72

[a] Addition can increase the number of significant figures.
[b] Subtraction can decrease the number of significant figures.
[c] 53.2 has 3 s.f. ⇒ need 3 s.f. in the answer ⇒ 1 in 1.726 is just place holder; need 3 digits to the right of decimal

Section Test

Questions
1. Which digits in 0.00303300 are significant?
2. You're using a graduated cylinder with mL markings to measure the volume of water. When you're ready to read the measurement, you see that meniscus fall between 29 and 30. How would you record that value?
3. How many significant digits should be in the answer to the following problem: (23.234 - 22.456) × 1.234?

Answers
1. First three 0s are not significant. All other are significant.
2. 29.5 mL (we approximate the last digit)
3. 3 significant digits because the subtraction leaves us with three significant digits.