Rounding Insignificant Figures

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by

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Abstract

This document provides rules for rounding insignificant figures from the results of mathematical calculations. After an introduction, the two main sections give examples to illustrate the rules for *addition and subtraction* and *multiplication and division*. For more complicated calculations, see the advanced topic document on propagating uncertainty. The fifth section provides guidance on reporting precision from the result of replicate measurements.

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I. Introduction

Performing calculations with a calculator or spreadsheet will return results with the number of significant figures that the device or program displays. When we report the results of scientific measurements, we must also report an indication of the uncertainty in those results. There is no point to report digits beyond what is known to be significant. Doing so can actually be misleading by implying that you know a result more precisely than you do.

As an example, let's say that you weigh an amount of caffeine to prepare a standard solution. The analytical balance can measure to 0.001 g and you weigh 0.554 g of caffeine. Dividing this amount by the formula weight of 194.19 g/mol on your calculator returns a molar amount of $2.852876049 \times 10^{-3}$ mol caffeine:

 $\frac{0.554 \text{ g}}{194.19 \text{ g/mol}} = 2.852876049 \times 10^{-3} \text{ mol}$

Retaining this number of significant figures in the final result is quite nonsensical and meaningless. It is up to you to round a result to properly reflect the uncertainty in a value.

The first step before rounding a result is to know the significance in the starting values. This point is discussed more fully in the next section, but as a start, we should write values to prevent confusion. Is the volume of 3300 mL known to four significant figures or only to two? Write values to make the number of significant figures clear by using scientific notation or prefixes in the units. If the volume 3300 mL is known to two significant figures, write it as 3.3×10^3 mL or 3.3 L. If it is known to four significant figures, then 3.300×10^3 mL or 3.300 L are appropriate representations.

Once we know how many significant figures we should report, we will round a value accordingly. I follow the "round-to-even" rule when rounding values that end in 5. For example, if the following values should be reported to only three significant figures, both 18.750 mL and 18.850 mL will round to 18.8 mL. The "round-to-even" rule reduces the likelihood of introducing a systematic bias, i.e., an overall increase in magnitude in a data set if all values ending in 5 are always rounded upward.

II. Expressing Uncertainty

In this document we only discuss the uncertainty in a result that is due to random variations in the repeatability of a measurement. The uncertainty due to repeatability is called the precision of a measurement. A common measure of precision, obtained by making replicate measurements, is the standard deviation. Determining a standard deviation takes a few key strokes on a calculator or writing a simple formula in a spreadsheet. Determining the accuracy of a measurement is a completely different issue. Accuracy, actually getting the right answer, requires extensive method validation experiments to determine the robustness of an analytical method. The uncertainty in the measurement of an unknown quantity is then inferred from the accuracy obtained when measuring known quantities. Method validation is beyond the scope of this document, but it should be clear that rounding to significant figures is only the first step in the larger task of describing the uncertainty in the result of a measurement or calculation.

If no precision is reported for a result, the uncertainty is generally assumed to be ± 1 in the least significant figure. As an example, reporting a mass of 0.554 g is the same as reporting (0.554 \pm 0.001) g. The experimenter believes that the true mass lies between 0.553 g and 0.555 g. If the uncertainty in the least significant figure is greater than ± 1 , it should be written explicitly with the value. The source of the reported uncertainty should be specified. If a precision is calculated, specify the method, e.g., standard deviation. Other sources of uncertainty might be an estimate based on observation or an estimate based on typical instrumental variations.

It is a common and acceptable practice to neglect significant figures through multi-step calculations and to then round the final result appropriately. If a calculation entails many steps, rounding after each step can help to keep track of significant figures. On a practical note, you can use <u>Format Cells</u>...' in a spreadsheet to display the appropriate number of significant figures in a calculated result.¹

III. Addition and Subtraction

When adding or subtracting numbers, the result should be rounded to the same number of significant figures as the operand in the calculation that is known to the least significance. It is easiest to see this concept if the values are written in a vertical column and aligned with the decimal point. As an example:

8.9444 g + 18.52 g ______27.4644 g

The correct rounded answer is: 27.46 g

The result of 27.46 g is rounded to the same decimal place as the factor in the addition that is known to the least precision, i.e., the 18.52 g value.

Subtraction follows the same procedure, for example:

¹ See Figures 4 through 7 in spreadsheet-help.pdf for examples.

The correct rounded answer is:

40.04 mV

In this case I do not ignore the last decimal place in the 5.007 mV value, but after completing the calculation I round the answer to match the precision of the 50.05 mV value.

When you have values with different units, it is best to convert them to common units. As an example, what is the total weight when 123.4 mg of an organic chemical is added to 10.05 g of KBr? Expressing both values in g and summing:

We see that we should round this result to 10.17 g. Try it yourself with the following practice exercises. Answers are at the end of this document.

Practice Exercises

- III.1. Sum the following weights: 4.223 g, 0.1751 g, and 11.05 g.
- III.2. Sum the total voltage: 1.38×10^{-2} V + 2.804×10^{-2} V + 4.365×10^{-3} V + 9.954×10^{-2} V.
- III.3. Sum the following potentials in a circuit: 0.050 V, 0.13 mV, −105 mV, 0.110 V, and −0.955 mV.
- III.4. 25.05 mL of CuSO₄ stock solution from a burette and 10 mL of NH₃ buffer from a graduated cylinder are transferred to a 50.0 mL volumetric flask. The flask is made up to the mark with distilled water and the flask is inverted several times to mix. What is the volume of solution in the flask?

IV. Multiplication and Division

The result of a multiplication or division operation will have the same number of significant figures as the factor(s) in the calculation with the smallest number of significant figures. For example:

Given that we know the weight to only three significant figures, the final result should be rounded to three significant figures:

2.85×10⁻³ mol

When multiplying or dividing by an integer, the integer is known exactly and does not limit the number of significant figures. For example, if the summation of four mass measurements (1.13, 0.98, 1.06, and 1.01 g) produces 4.18 g. The mean of these measurements is:

 $\frac{4.18 \text{ g}}{4}$ = 1.04500 g

Using our rules, we truncate this result to 1.04 g.

The summation of four different mass measurements (4.95, 4.97, 4.96, and 4.95 g) produces 19.83 g. The mean of these measurements is:

$$\frac{19.83 \text{ g}}{4}$$
 = 4.95750 g

The total mass now has four significant figures, so using our rules, we truncate this result to 4.958 g. However doing so overestimates the precision given that the individual measurements were made only to two decimal places. We will see in the next section that a better way to treat replicate data is to use statistical measures of precision such as the standard deviation, *s*.

An exponent on a variable is shorthand for another operation, so it does not enter into determining the number of significant figures in a result. The following calculation of the area of a circular microelectrode illustrates this point. This example includes another case of an integer value, which is known exactly, and doesn't reduce the significant figures in the result. If the electrode diameter is 3.0 mm, the radius, *r*, is:

$$r = \frac{3.0 \text{ mm}}{2} = 1.5 \text{ mm}$$

The 2 is an integer and known exactly. The 1.5 mm result maintains the same number of significant figures as the 3.0 mm operand. The area, *A*, is:

 $A = \pi r^2$

We use a value for pi that has more significant figures than the other operands. The calculation and rounded result is:

A = (3.1416)(1.5 mm)² = (3.1416)(1.5 mm)(1.5 mm) = 7.0686 mm² = 7.1 mm² Square roots can be a little tricky. We want the result to give us the same answer when taken in reverse. The square root of 7.0 is:

Rounding to the same number of significant figures as the 7.0 gives us a result of 2.6. However, squaring 2.6 gives 6.8, so we report the $(7.0)^{1/2}$ = 2.65. Squaring 2.65 returns the value of 7.0:

 $(2.65)^2 = 7.0.$

Practice Exercises

- IV.1. What is the density of a salt solution if 5.00 mL of the solution weighed 5.1234 g?
- IV.2. What is the usable surface area, A, of a Pt wire electrode that is 1.0 mm in diameter and 10.0 mm in length? The wire has a circular cross-section. Note that one end of the electrode is connected to an electrical circuit and is not in contact with the test solution.
- IV.3. 1.05 g and 250.41 mg of caffeine are added to a volumetric flask. How many moles of caffeine are present in the flask? The formula weight of caffeine is 194.19 g mol⁻¹.

V. Replicate Measurements

Analysts make replicate measurements to provide greater confidence that results are not inaccurate due to mistakes. Random errors will average out to some extent. If a gross error occurs for one trial, it will be apparent as an outlier in the data set. Obviously making a systematic error in all trials introduces a bias in the final result, and we rely on method validation experiments to know that we can make accurate measurements.

When the random variation in replicate measurements is larger than the number of significant figures of an individual measurement, the repeatability will determine the number of significant figures to retain in the result. Let's revisit the previous examples of finding average values.

Dividing by four and rounding gave 4.958 g.

Now however let's enter these values into a spreadsheet		А	В	С
or calculator and find the average and standard deviation.			weight	
The result is shown in the adjacent table.	1	_	(g)	
	2		4.95	
The standard deviation shows the random variability to	3		4.97	
be ±0.01 g, so the correct way to report this average is:	4		4.96	
(4.96 ± 0.01) g or simply 4.96 g.	5		4.95	
	6	sum	19.83	g
	7	avg	4.95750	g
	8	stdev	0.00957	g
Performing the same calculation for our other averaging		А	В	С
example (see adjacent table), the standard deviation			weight	
shows the random variability to be ± 0.07 g, so the correct	9		(g)	_
way to report this average is:	10		1.13	
(1.04 ± 0.07) g.	11		0.98	
	12		1.06	
When comparing results of different magnitude, it is use-	13		1.01	_
ful to express the uncertainty on a relative basis. The fol-	14	sum	4.18	g
lowing calculations express the repeatability in a relative	15	avg	1.04500	g
basis, where	16	stdev	0.06557	g

RSD is relative standard deviation.

<u>0.07 g</u> 1.04 g × 100% = 7% RSD $\frac{0.01 \text{ g}}{4.96 \text{ g}}$ × 100% = 0.2% RSD

The two results above are each known to three significant figures, but the %-RSD values show that the repeatability of the two measurements was quite different. The following measurements and calculations provide more illustration of considerations for reporting uncertainties.

The density of isooctane (2) trimethyl-pentane) was measured weighing 5.00-mL aliquots delive with a volumetric pipet. The pipet class A and has a listed toleranc ±0.01 mL. 1 part in 500 is equiva to a precision of 0.2 %.

The tables to the right show the

,2,4-	isooctane (student 1)		
d by	weight (g)	density (g/mL)	
ered	3.4383	0.68766	
was	3.4451	0.68902	
e of	3.4366	0.68732	
alent	3.442	0.6884	
	3.4315	0.6863	
	3.4353	0.68706	

measurement results and spreadsheet calculations of density in g/mL. The volume is known to 5.00 mL, or three significant figures. After dividing the weight by this value the result should be reported to three significant figures. For student 1, the average result is:

octane at 24 C, the measured solution

Data from student 2 shows more variation. In this case, the repeatability and not the pipet tolerance is not the limiting factor in the precision that can be reported for these measurements. In this case we can report:

avg	0.687627
std	0.000971
%-RSD	0.141233

ures. For student 1, the average result	i	isooctane (stud	lent 2)
is:		net wt (g)	density (g/mL)
		3.417	0.6834
0.688 ± 0.001 g/mL		3.286	0.6572
		3.278	0.6556
Given that the tolerance of the pipet		3.437	0.6874
is not as precise as this result, I will		3.433	0.6866
report a more conservative:		3.437	0.6874
0.688 ± 0.002 g/mL	avg		0.676267
	stdev		0.015467
This result is quite close to the ex- pected density of 0.689 g/mL for iso-	%-RSD		2.287185

0.67₆ ± 0.01₅ g/mL or 0.68 ± 0.02 g/mL

temperature.

VI. Answers to Practice Exercises

Addition and Subtraction

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III.1. Sum the following weights: 4.223 g, 0.1751 g, and 11.05 g.
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Aligning the values in a vertical column:

4.223 g

0.1751 g

11.05 g

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15.448 g

We see that we should round the result to the same signifi-

cance as the 11.05 g value: 15.45 g.
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III.2. Sum the total voltage: 1.38×10^{-2} V + 2.804×10^{-2} V + 4.365×10^{-3} V + 9.954×10^{-2} V.

For clarity I'll convert from scientific notation to decimal spaces and again align vertically:

Round answer to the same significance as the 0.0138 V value: 0.1457 V. Even though 0.0138 V had only three significant figures,

since the sum increased in magnitude we ended up with four significant figures.

III.3. Sum the following potentials in a circuit: 0.050 V, 0.13 mV, -105 mV, 0.110 V, and -0.955 mV.

Convert all values to the same units and then proceed as before. Working in either mV or V will give the same result:

0.050	V	50	mV
0.00013	V	0.13	mV
-0.105	V	-105	mV
0.110	V	110	mV
-0.000955	V	-0.955	mV
0.054175	V	54.175	mV

Correct sums are:

0.054 V or 54 mV

III.4. 25.05 mL of CuSO₄ stock solution from a burette and 11 mL of NH₃ buffer from a graduated cylinder are transferred to a class B, 50.0-mL volumetric flask. The flask is made up to the mark with distilled water and the flask is inverted several times to mix. What is the volume of solution in the flask?

The volume is **50.0 mL**. The precision in the volume additions to the flask do not affect this result. The uncertainty depends only on the accuracy of the flask and the skill of the analyst using it. This example illustrates the need to know the context of a calculation to report the result correctly.

Multiplication and Division

IV.1. What is the density, ρ , of a salt solution if 5.00 mL of the solution weighed 5.1234 g?

$$\frac{\rho}{=} \frac{5.1234 \text{ g}}{5.00 \text{ mL}} = 1.024680 \text{ g/mL}$$

Since the volume is known to only three significant figures, rounding the result to three significant figures gives:

 $\frac{\rho}{=}$ 1.02 g/mL

IV.2. What is the usable surface area, A, of a Pt wire electrode that is 1.0 mm in diameter and 10.0 mm in length? The wire has a circular cross-section. Note that one end of the electrode is connected to an electrical circuit and is not in contact with the test solution.

The surface area of a cylindrical electrode in contact with solution is the area along the length of the wire plus one end surface:

 $A = 2\pi rh + \pi r^2$

The radius is one-half of the diameter and we retain the two significant figures known for the diameter:

 $r = \frac{1.0 \text{ mm}}{2} = 0.50 \text{ mm}$

Likewise when we square the 0.50 mm the result will have two significant figures:

 $r^2 = (0.50 \text{ mm}) (0.50 \text{ mm}) = 0.25 \text{ mm}^2$.

The full expression is a combination of multiplication and addition. Complete the multiplication steps before round-ing:

 $A = 2(3.1416)(0.50 \text{ mm})(10.0 \text{ mm}) + (3.1416)(0.50 \text{ mm})^2$

Each term in the sum should be rounded to two significant figures, so the first term will determine the number of decimal places to show in the result. I show the extra decimal places for you to check your result if you are working along:

 $A = 31.416 \text{ mm}^2 + 0.785 \text{ mm}^2$

The final result on rounding is:

 $A = 32 \text{ mm}^2$

IV.3. 1.05 g and 250.4 mg of caffeine are added to a volumetric flask. How many moles of caffeine are present in the flask? The formula weight of caffeine is 194.19 g mol⁻¹.

In multistep calculations, perform addition and subtractions operations first:

This intermediate result is rounded to 1.30 g. Now do the division:

Rounding to three significant figures gives 6.69×10^{-3} mol caffeine.