(b) Apply Equation 4-15 to get

$$\frac{s_y}{y} = 2.303 \times (0.003) = 0.0069$$

$$s_y = 0.0069y = 0.0069 \times 15.849 = 0.11$$

Therefore,

$$y = \text{antilog}[1.200(\pm 0.003)] = 15.8 \pm 0.1$$

(c) $$\frac{s_y}{y} = 2.303 \times (0.3) = 0.69$$

$$s_y = 0.69y = 0.69 \times 2.5119 \times 10^{45} = 1.7 \times 10^{45}$$

Thus,

$$y = \text{antilog}[45.4(\pm 0.3)] = 2.5(\pm 1.7) \times 10^{45} = 3(\pm 2) \times 10^{45}$$

Example 4-4C demonstrates that a large absolute error is associated with the antilogarithm of a number with few digits beyond the decimal point. This large uncertainty is due to the fact that the numbers to the left of the decimal (the *characteristic*) serve only to locate the decimal point. The large error in the antilogarithm results from the relatively large uncertainty in the *mantissa* of the number (that is, 0.4 ± 0.3).

4D Reporting Computed Data

A numerical result is worthless to users of the data unless they know something about its quality. Therefore, it is essential to indicate your best estimate of the reliability of your data. One of the best ways of indicating reliability is to give a confidence interval at the 90% or 95% confidence level, as we describe in Section 5A-2. Another method is to report the absolute standard deviation or the coefficient of variation of the data. If one of these is reported, it is a good idea to indicate the number of data points that were used to obtain the standard deviation so that the user has some idea of the reliability of *s*. A much less satisfactory but more common indicator of the quality of data is the **significant figure convention**.

The **significant figures** in a number are all the certain digits plus the first uncertain digit.

4D-1 Significant Figures

We often indicate the probable uncertainty associated with an experimental measurement by rounding the result so that it contains only **significant figures**. By convention, the significant figures in a number are all the certain digits *plus the first uncertain digit*. For example, when you read the 50-mL buret section shown in **Figure 4-5**, you can easily tell that the liquid level is greater than 31.0 mL and less than 30.9 mL. You can also estimate the position of the liquid between the graduations to about 0.02 mL. So, using the significant figure convention, you should report the volume delivered as 30.96 mL, which has four significant figures. Note that the first three digits are certain, and the last digit (6) is uncertain.

A zero may or may not be significant depending on its location in a number. A zero that is surrounded by other digits is always significant (such as in 30.96 mL) because it is read directly and with certainty from a scale or instrument readout. On the other hand, zeros that only locate the decimal point for us are not. If we write 30.96 mL as 0.03096 L, the number of significant figures is the same. The only

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FIGURE 4-5
A buret section showing the liquid level and meniscus.

Rules for determining the number of significant figures:
1. Disregard all initial zeros.
2. Disregard all final zeros *unless they follow a decimal point.*
3. All remaining digits including zeros between nonzero digits are significant.

function of the zero before the 3 is to locate the decimal point, so it is not significant. Terminal, or final, zeros may or may not be significant. For example, if the volume of a beaker is expressed as 2.0 L, the presence of the zero tells us that the volume is known to a few tenths of a liter so that both the 2 and the zero are significant figures. If this same volume is reported as 2000 mL, the situation becomes confusing. The last two zeros are not significant because the uncertainty is still a few tenths of a liter or a few hundred milliliters. In order to follow the significant figure convention in a case such as this, use scientific notation and report the volume as 2.0×10^3 mL.

4D-2 Significant Figures in Numerical Computations

Determining the appropriate number of significant figures in the result of an arithmetic combination of two or more numbers requires great care.[4]

Sums and Differences

For addition and subtraction, the number of significant figures can be found by visual inspection. For example, in the expression

$$3.4 + 0.020 + 7.31 = 10.730$$
$$= 10.7 \text{ (rounded)}$$

the second and third decimal places in the answer cannot be significant because 3.4 is uncertain in the first decimal place. Hence, the result should be rounded to 10.7. We can generalize and say that, for addition and subtraction, the result should have the same number of decimal places as the number with the *smallest* number of decimal places. Note that the result contains three significant digits even though two of the numbers involved have only two significant figures.

Products and Quotients

Express data in scientific notation to avoid confusion in determining whether terminal zeros are significant.

As a rule of thumb, for addition and subtraction, the result should contain the same number of decimal places as the number with the *smallest* number of decimal places.

When adding and subtracting numbers in scientific notation, express the numbers to the same power of 10. For example,

$$\begin{aligned} 2.432 \times 10^6 &= 2.432 \times 10^6 \\ +6.512 \times 10^4 &= +0.06512 \times 10^6 \\ -1.227 \times 10^5 &= -0.1227 \times 10^6 \\ & 2.37442 \times 10^6 \\ &= 2.374 \times 10^6 \text{ (rounded)} \end{aligned}$$

The weak link for multiplication and division is the number of *significant figures* in the number with the smallest number of significant figures. *Use this rule of thumb with caution.*

Sometimes it is suggested for multiplication and division that the answer should be rounded so that it contains the same number of significant digits as the original number with the smallest number of significant digits. Unfortunately, this procedure sometimes leads to incorrect rounding. For example, consider the two calculations

$$\frac{24 \times 4.52}{100.0} = 1.08 \quad \text{and} \quad \frac{24 \times 4.02}{100.0} = 0.965$$

If we follow the suggestion, the first answer would be rounded to 1.1 and the second to 0.96. A better procedure is to assume unit uncertainty in the last digit of each number. For example, in the first quotient, the relative uncertainties associated with each of these numbers are 1/24, 1/452, and 1/1000. Because the first relative uncertainty is much larger than the other two, the relative uncertainty in the result is also 1/24; the absolute uncertainty is then

$$1.08 \times \frac{1}{24} = 0.045 \approx 0.04$$

By the same argument, the absolute uncertainty of the second answer is given by

$$0.965 \times \frac{1}{24} = 0.040 \approx 0.04$$

Therefore, the first result should be rounded to three significant figures or 1.08, but the second should be rounded to only two, that is, 0.96.

[4]For an extensive discussion of propagation of significant figures, see L. M. Schwartz, *J. Chem. Educ.*, **1985**, *62*, 693, **DOI**: 10.1021/ed062p693.

Logarithms and Antilogarithms

Be especially careful in rounding the results of calculations involving logarithms. The following rules apply to most situations and are illustrated in Example 4-7:

1. In a logarithm of a number, keep as many digits to the right of the decimal point as there are significant figures in the original number.
2. In an antilogarithm of a number, keep as many digits as there are digits to the right of the decimal point in the original number.[5]

> The number of significant figures in the *mantissa*, or the digits to the right of the decimal point of a logarithm, is the same as the number of significant figures in the original number. Thus, $\log(9.57 \times 10^4) = 4.981$. Since 9.57 has three significant figures, there are three digits to the right of the decimal point in the result.

EXAMPLE 4-7

Round the following answers so that only significant digits are retained: (a) $\log 4.000 \times 10^{-5} = -4.3979400$ and (b) $\text{antilog } 12.5 = 3.162277 \times 10^{12}$

Solution

(a) Following rule 1, retain four digits to the right of the decimal point

$$\log 4.000 \times 10^{-5} = -4.3979$$

(b) Following rule 2, retain only one digit

$$\text{antilog } 12.5 = 3 \times 10^{12}$$

4D-3 Rounding Data

Always round the computed results of a chemical analysis in an appropriate way. For example, consider the replicate results: 41.60, 41.46, 41.55, and 41.61. The mean of this data set is 41.555, and the standard deviation is 0.069. When we round the mean, do we take 41.55 or 41.56? A good guide to follow when rounding a 5 is always to round to the nearest even number. In this way, we eliminate any tendency to round in a fixed direction. In other words, there is an equal likelihood that the nearest even number will be the higher or the lower in any given situation. Accordingly, we might choose to report the result as 41.56 ± 0.07. If we have reason to doubt the reliability of the estimated standard deviation, we might report the result as 41.6 ± 0.1.

> In rounding a number ending in 5, always round so that the result ends with an even number. Thus, 0.635 rounds to 0.64 and 0.625 rounds to 0.62.

Note that *it is seldom justifiable to keep more than one significant figure in the standard deviation* because the standard deviation contains error as well. For certain specialized purposes, such as reporting uncertainties in physical constants in research articles, it may be useful to keep two significant figures, and there is certainly nothing wrong with including a second digit in the standard deviation. However, it is important to recognize that the uncertainty usually lies in the first digit.

> Always keep in mind that you are seldom justified in keeping more than one digit in the standard deviation, particularly when N is 5 or fewer.

4D-4 Expressing Results of Chemical Calculations

Two cases are encountered when reporting the results of chemical calculations. If the standard deviations of the values making up the final calculation are known, apply the propagation of error methods discussed in Section 4C and round the results to contain significant digits. However, if we are asked to perform calculations where the precision is indicated only by the significant figure convention, common sense assumptions must be made as to the uncertainty in each number. With these assumptions, the uncertainty of the final result is then estimated using the methods presented in Section 4C. Finally, the result is rounded so that it contains only significant digits.

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[5]D. E. Jones, *J. Chem. Educ.*, **1971**, *49*, 753, **DOI**: 10.1021/ed049p753.

It is especially important to postpone rounding until the calculation is completed. At least one extra digit beyond the significant digits should be carried through all the computations in order to avoid a *rounding error*. This extra digit is sometimes called a "guard" digit. Modern calculators generally retain several extra digits that are not significant, and the user must be careful to round final results properly so that only significant figures are included. Example 4-8 illustrates this procedure.

EXAMPLE 4-8

A 3.4842-g sample of a solid mixture containing benzoic acid, C_6H_5COOH (122.123 g/mol), was dissolved and titrated with base to a phenolphthalein end point (see Chapter 12 for titration procedures). The acid consumed 41.36 mL of 0.2328 M NaOH. Calculate the percent benzoic acid (HBz) in the sample.

Solution

As shown in Section 11C-3, the calculation takes the following form:

$$\%\text{HBz} = \frac{41.36\ \cancel{\text{mL NaOH}} \times 0.2328\ \dfrac{\cancel{\text{mmol NaOH}}}{\cancel{\text{mL}}} \times \dfrac{1\ \cancel{\text{mmol HBz}}}{\cancel{\text{mmol NaOH}}} \times \dfrac{122.123\ \text{g HBz}}{1000\ \cancel{\text{mmol HBz}}}}{3.842\ \text{g sample}}$$

$$\times\ 100\%$$
$$= 30.606\%$$

Since all operations are either multiplication or division, the relative uncertainty of the answer is determined by the relative uncertainties of the experimental data. We can estimate what these uncertainties are.

1. The position of the liquid level in a buret can be estimated to ± 0.02 mL (Figure 4-5). In reading the buret, two readings (initial and final) must be made so that the standard deviation of the volume s_V will be

$$s_V = \sqrt{(0.02)^2 + (0.02)^2} = 0.028 \text{ mL}$$

The relative uncertainty in volume s_V/V is then

$$\frac{s_V}{V} = \frac{0.028}{41.36} \times 1000 \text{ ppt} = 0.68 \text{ ppt}$$

2. Generally, the absolute uncertainty of a mass obtained with an analytical balance will be on the order of ± 0.0001 g. Thus, the relative uncertainty of the denominator s_D/D is

$$\frac{0.0001}{3.4842} \times 1000 \text{ ppt} = 0.029 \text{ ppt}$$

3. Usually, we can assume that the absolute uncertainty in the concentration of a reagent solution is ± 0.0001 M, and so the relative uncertainty in the concentration of NaOH, s_c/c, is

$$\frac{s_c}{c} = \frac{0.0001}{0.2328} \times 1000 \text{ ppt} = 0.43 \text{ ppt}$$

4. The relative uncertainty in the molar mass of HBz is several orders of magnitude smaller than any of the three experimental values and will not be significant. Note, however, that we should retain enough digits in the calculation so that the molar mass is given to at least one more digit (the guard digit) than any of the experimental data. Thus, in the calculation, use 122.123 for the molar mass (carrying two extra digits in this instance).

(*continued*)